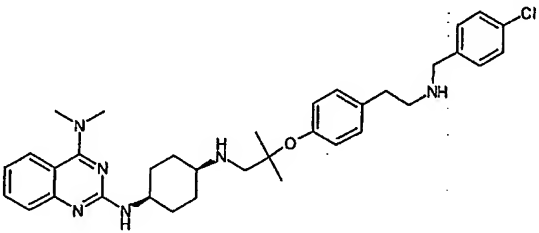
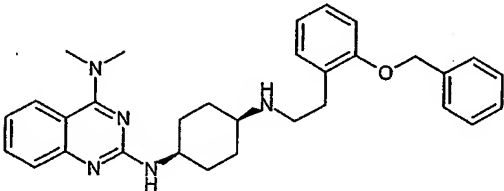
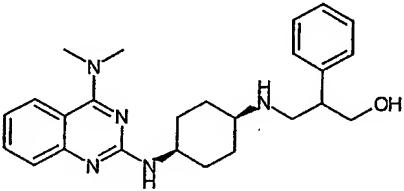
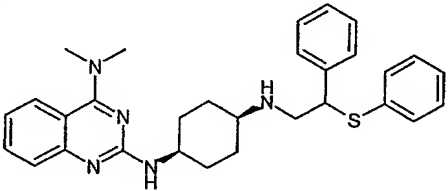
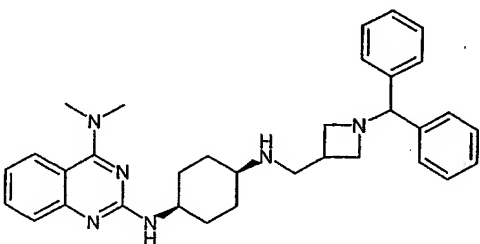
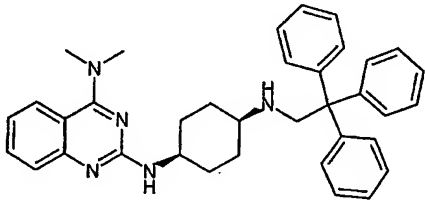
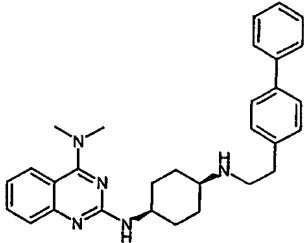
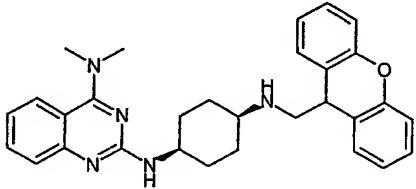
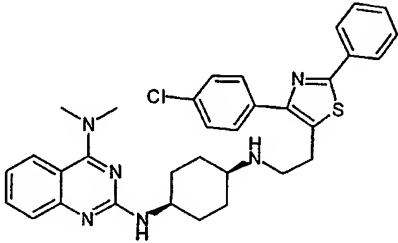
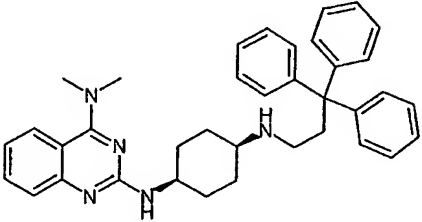
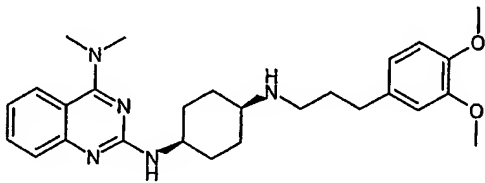
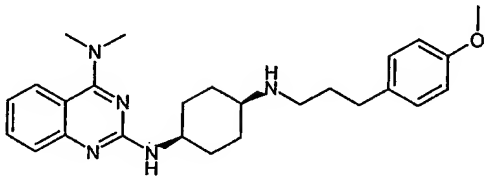
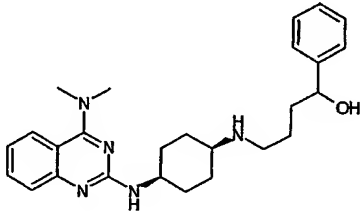
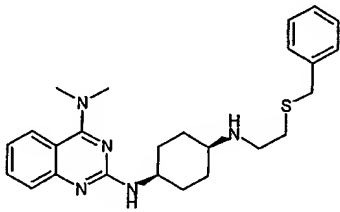
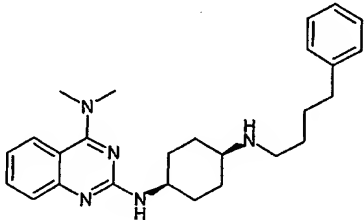
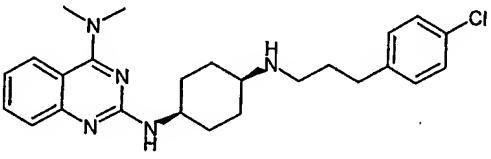
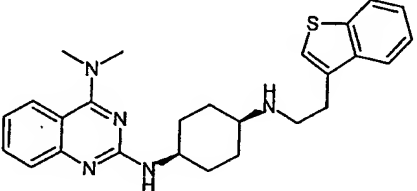
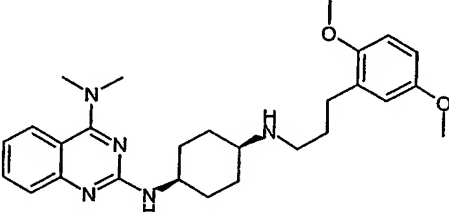
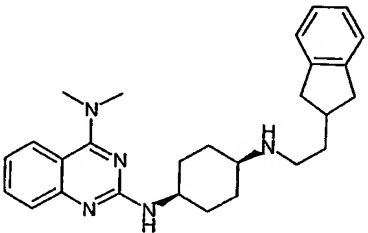
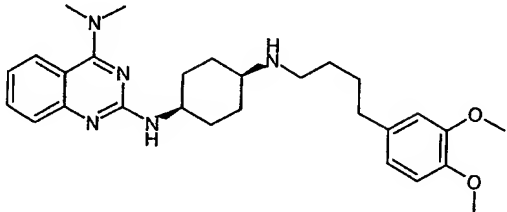
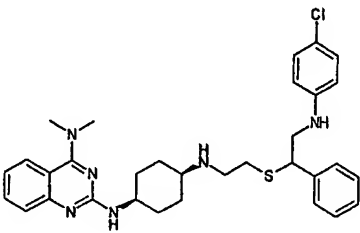
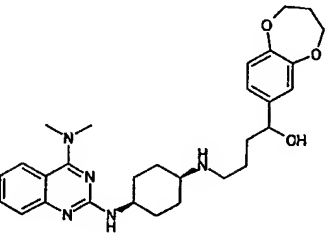
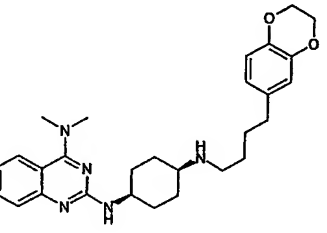
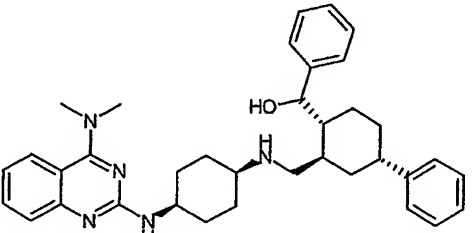
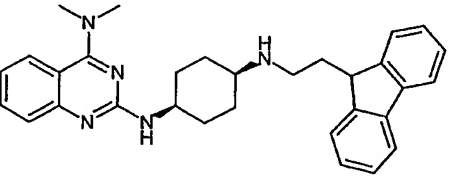


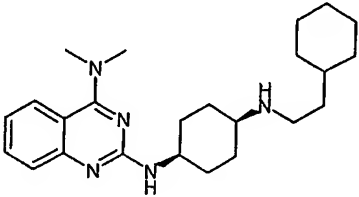
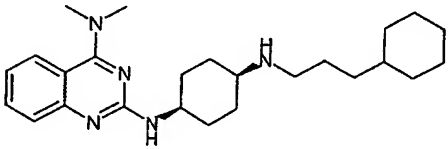
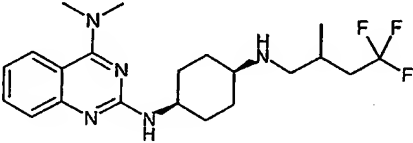
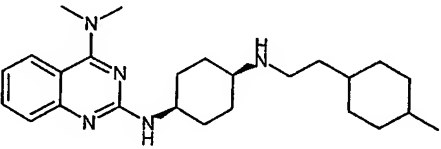
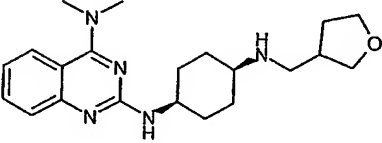
Example No.	Structure	APCI-MS
1522		601 (M + H)
1523		496 (M + H)
1524		420 (M + H)
1525		498 (M + H)
1526		521 (M + H)

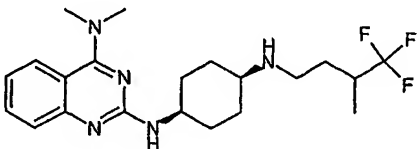
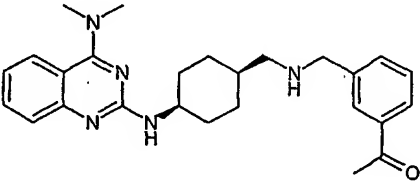
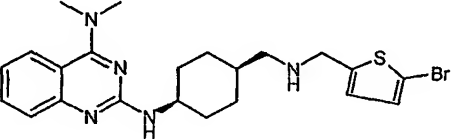
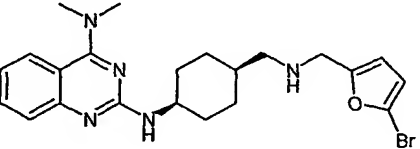
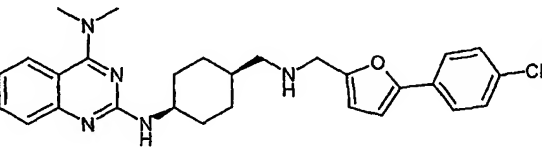
Example No.	Structure	APCI-MS
1527		542 (M + H)
1528		466 (M + H)
1529		480 (M + H)
1530		583 (M + H)
1531		556 (M + H)

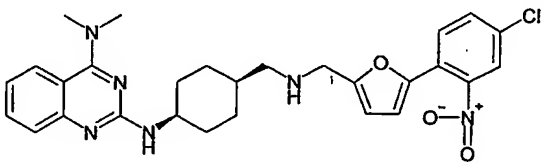
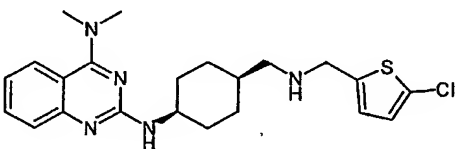
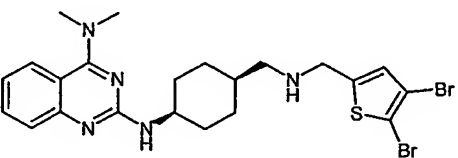
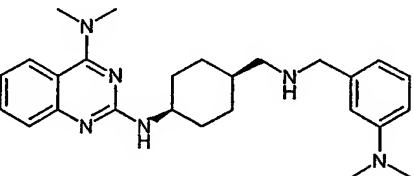
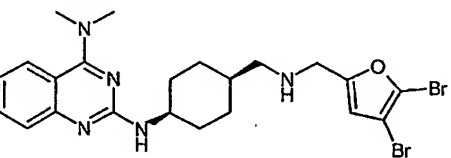
Example No.	Structure	APCI-MS
1532		464 (M + H)
1533		434 (M + H)
1534		434 (M + H)
1535		436 (M + H)
1536		418 (M + H)

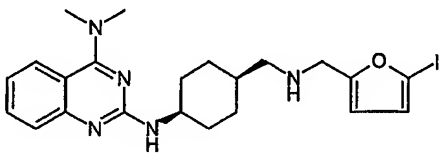
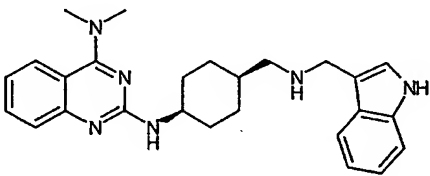
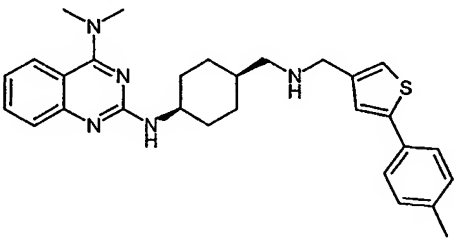
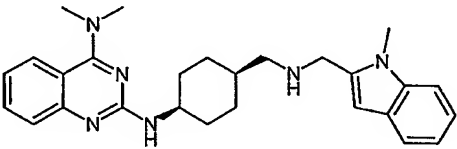
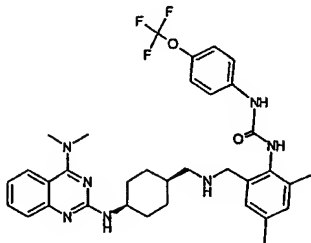
Example No.	Structure	APCI-MS
1537		438 (M + H)
1538		446 (M + H)
1539		464 (M + H)
1540		430 (M + H)
1541		478 (M + H)

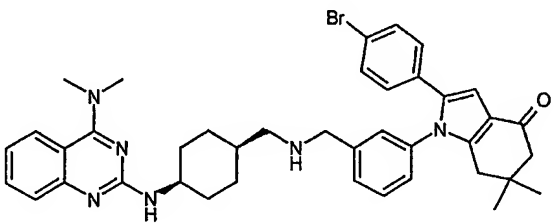
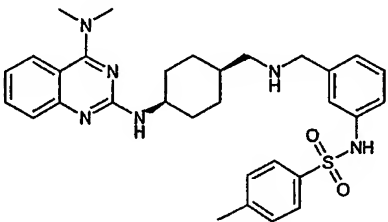
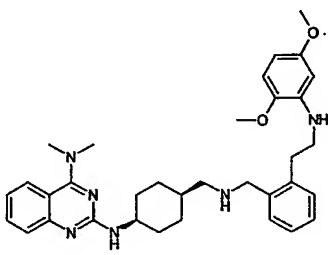
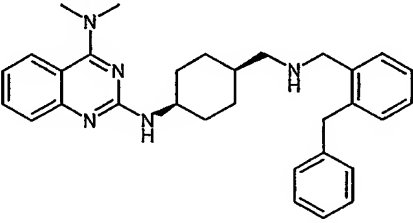
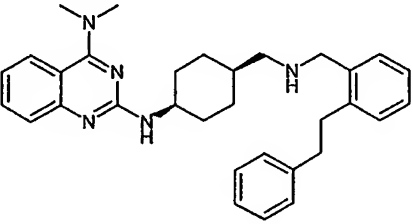
Example No.	Structure	APCI-MS
1542		575 (M + H)
1543		506 (M + H)
1544		476 (M + H)
1545		564 (M + H)
1546		478 (M + H)

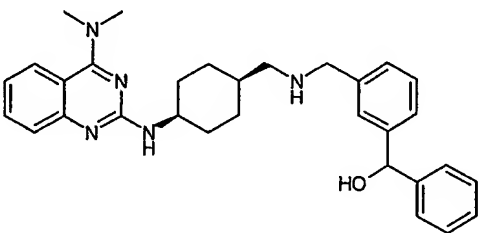
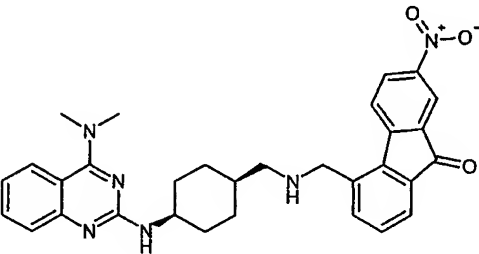
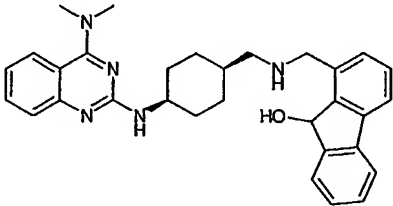
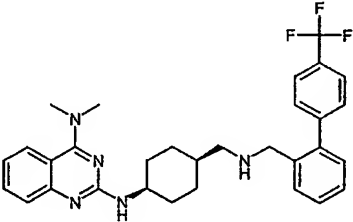
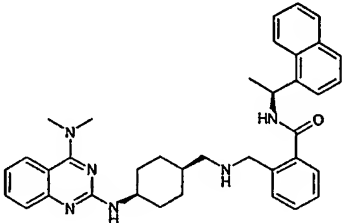
Example No.	Structure	APCI-MS
1547		396 (M + H)
1548		410 (M + H)
1549		410 (M + H)
1550		410 (M + H)
1551		370 (M + H)

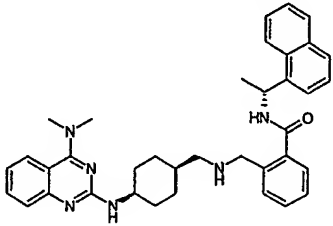
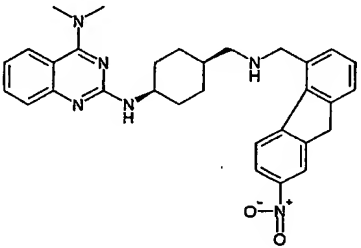
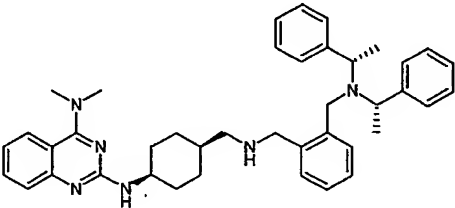
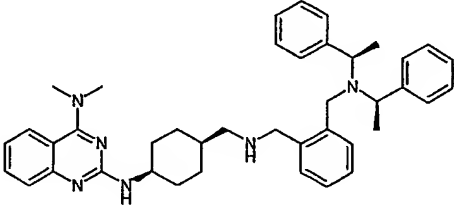
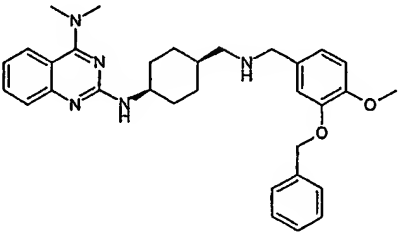
Example No.	Structure	APCI-MS
1552		410 (M + H)
1553		432 (M + H)
1554		474 (M + H)
1555		458 (M + H)
1556		490 (M + H)

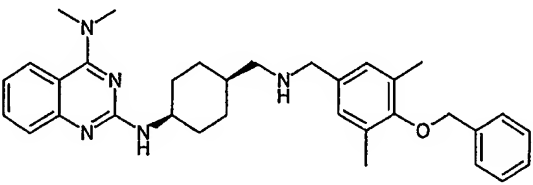
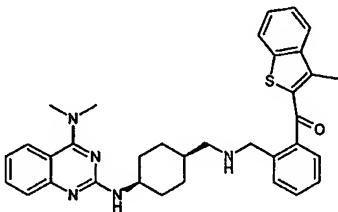
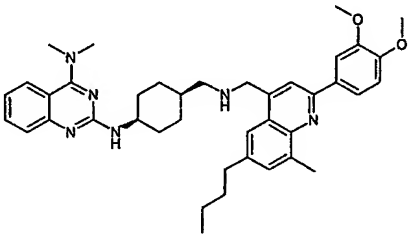
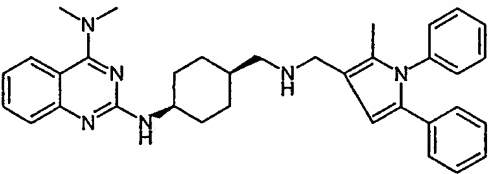
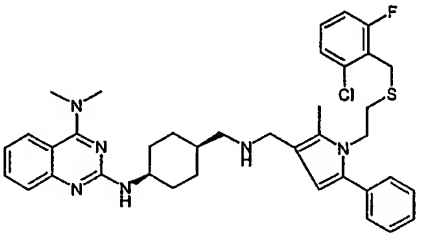
Example No.	Structure	APCI-MS
1557		535 (M + H)
1558		430 (M + H)
1559		552 (M + H)
1560		433 (M + H)
1561		536 (M + H)

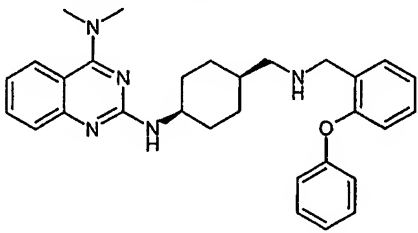
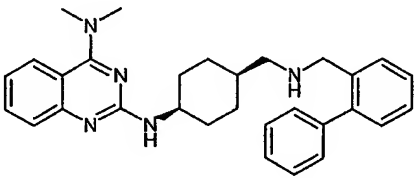
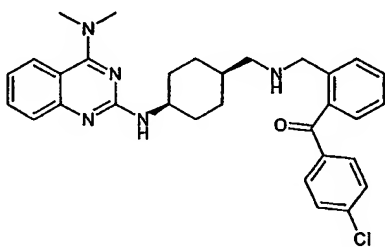
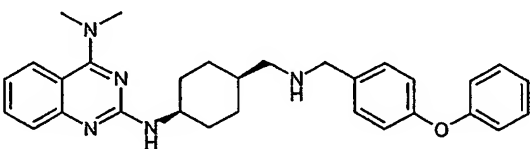
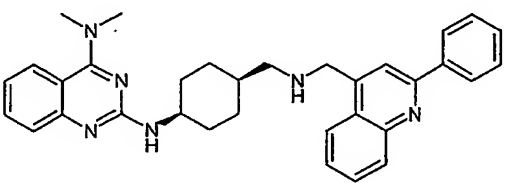
Example No.	Structure	APCI-MS
1562		506 (M + H)
1563		429 (M + H)
1564		486 (M + H)
1565		443 (M + H)
1566		636 (M + H)

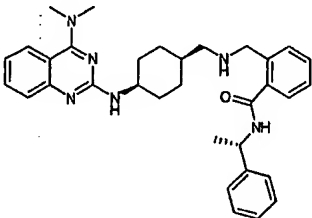
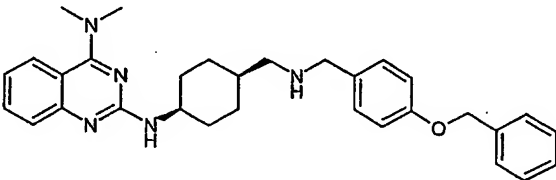
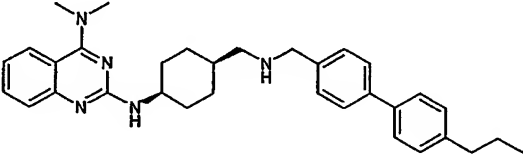
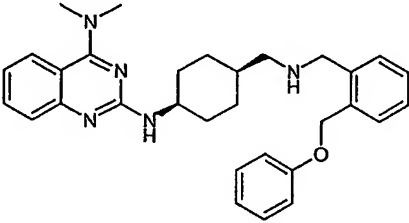
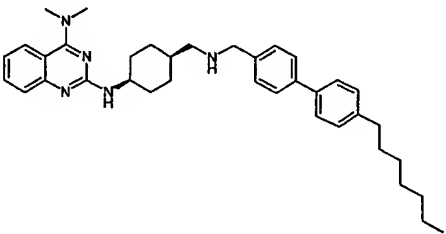
Example No.	Structure	APCI-MS
1567		705 (M + H)
1568		559 (M + H)
1569		569 (M + H)
1570		480 (M + H)
1571		494 (M + H)

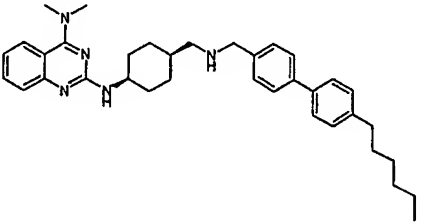
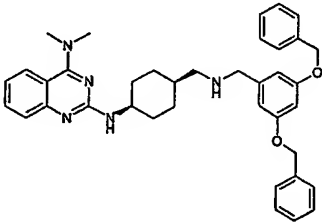
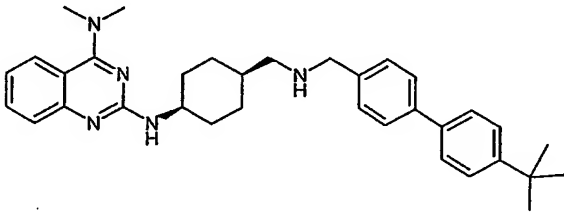
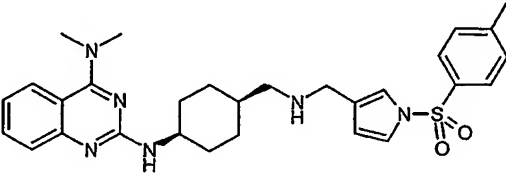
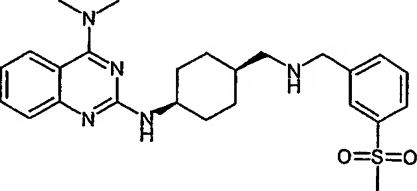
Example No.	Structure	APCI-MS
1572		496 (M + H)
1573		537 (M + H)
1574		494 (M + H)
1575		534 (M + H)
1576		587 (M + H)

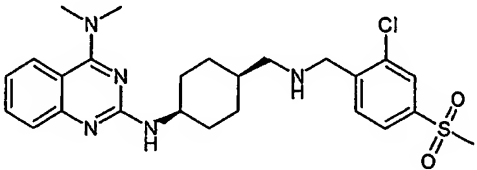
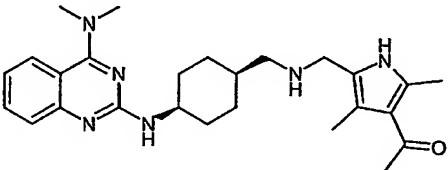
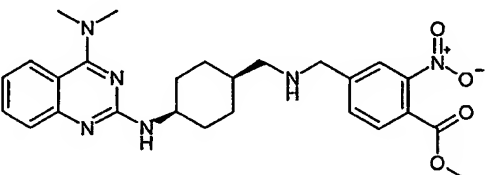
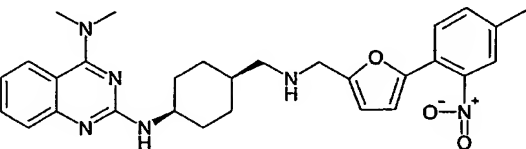
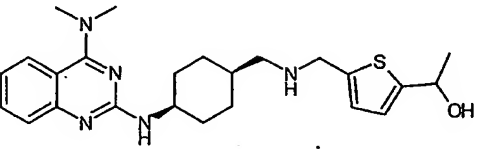
Example No.	Structure	APCI-MS
1577		587 (M + H)
1578		523 (M + H)
1579		627 (M + H)
1580		627 (M + H)
1581		526 (M + H)

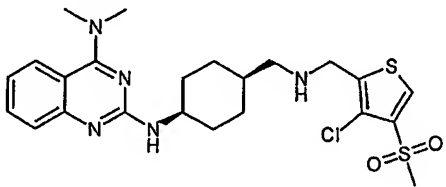
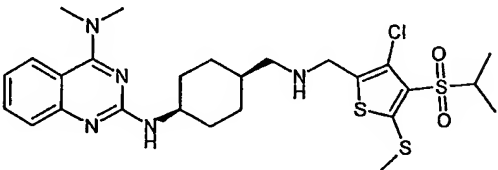
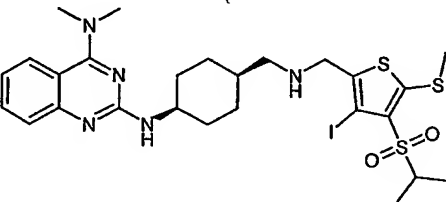
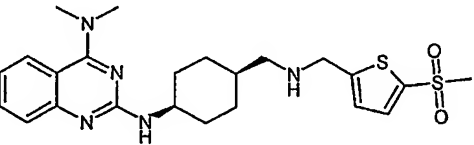
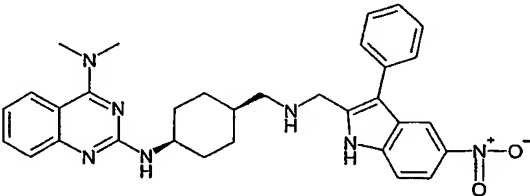
Example No.	Structure	APCI-MS
1582		524 (M + H)
1583		564 (M + H)
1584		647 (M + H)
1585		545 (M + H)
1586		671 (M + H)

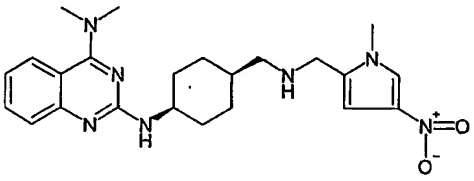
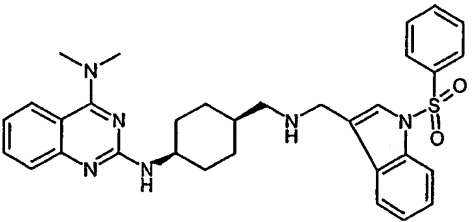
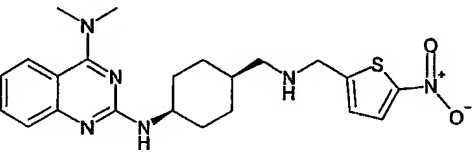
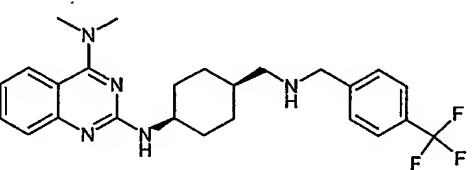
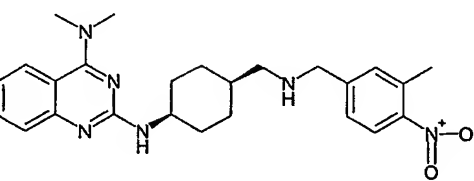
Example No.	Structure	APCI-MS
1587		482 (M + H)
1588		466 (M + H)
1589		528 (M + H)
1590		482 (M + H)
1591		517 (M + H)

Example No.	Structure	APCI-MS
1592		537 (M + H)
1593		496 (M + H)
1594		508 (M + H)
1595		496 (M + H)
1596		564 (M + H)

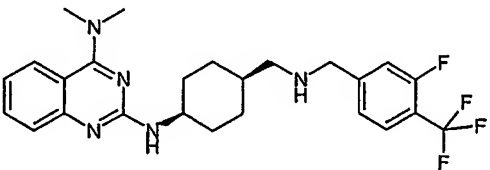
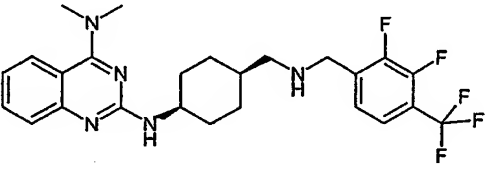
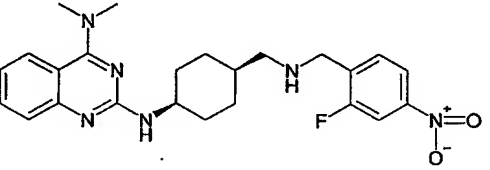
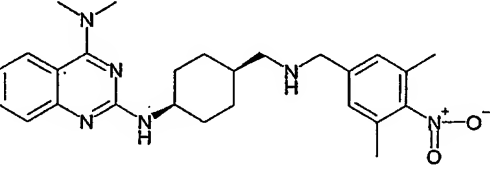
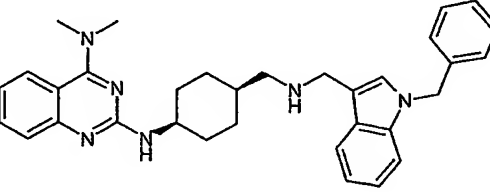
Example No.	Structure	APCI-MS
1597		550 (M + H)
1598		602 (M + H)
1599		522 (M + H)
1600		533 (M + H)
1601		468 (M + H)

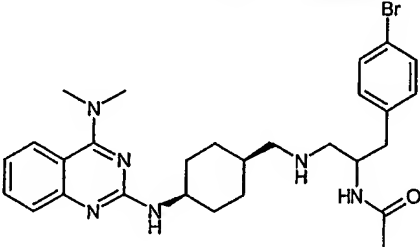
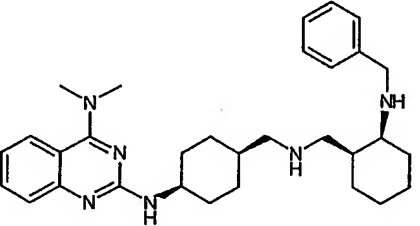
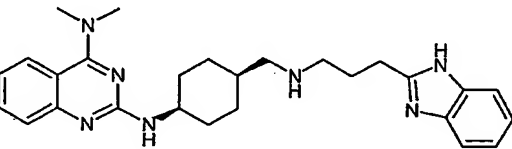
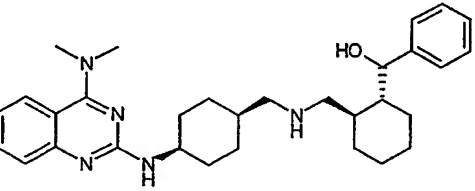
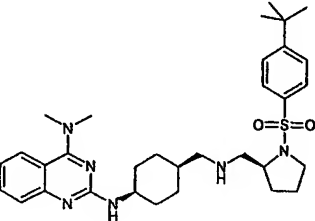
Example No.	Structure	APCI-MS
1602		502 (M + H)
1603		449 (M + H)
1604		493 (M + H)
1605		515 (M + H)
1606		440 (M + H)

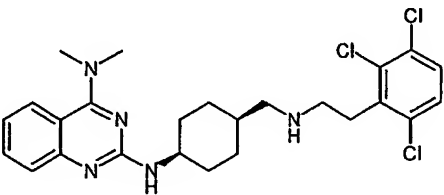
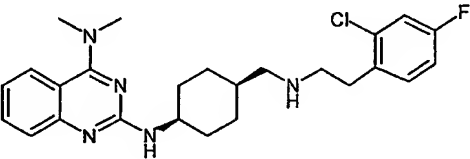
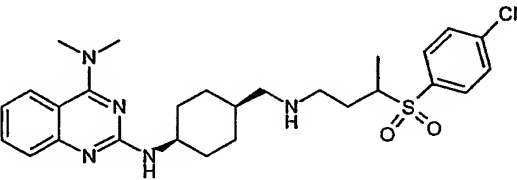
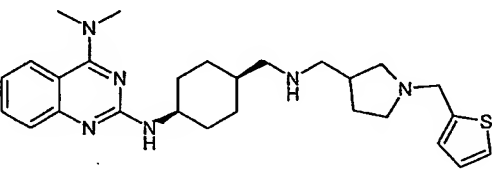
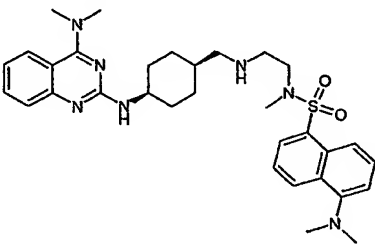
Example No.	Structure	APCI-MS
1607		508 (M + H)
1608		582 (M + H)
1609		674 (M + H)
1610		474 (M + H)
1611		548 (M - H)

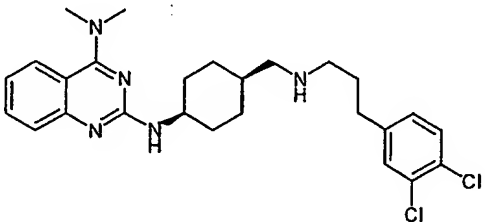
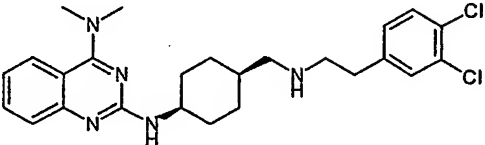
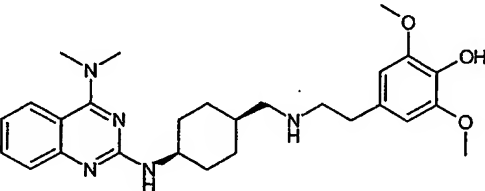
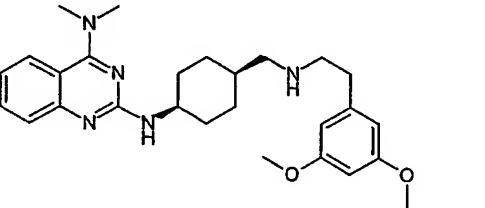
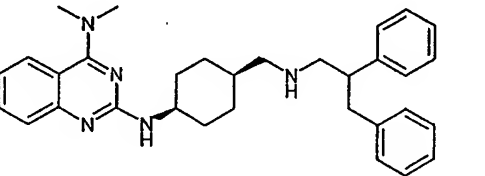
Example No.	Structure	APCI-MS
1612		438 (M + H)
1613		569 (M + H)
1614		441 (M + H)
1615		458 (M + H)
1616		449 (M + H)

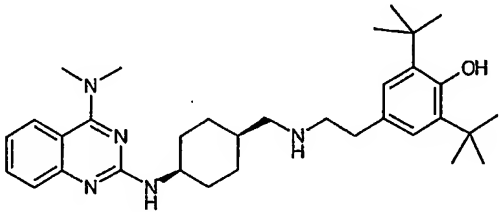
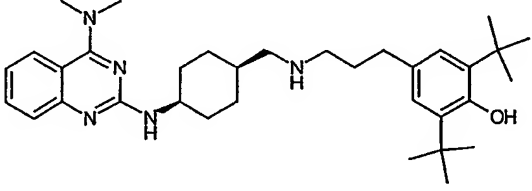
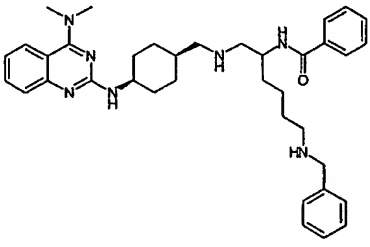
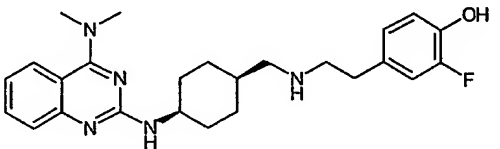
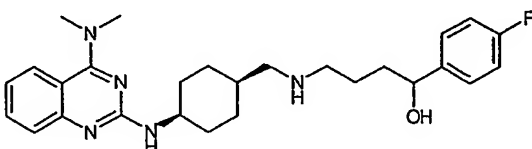
Example No.	Structure	APCI-MS
1617		435 (M + H)
1618		465 (M + H)
1619		476 (M + H)
1620		526 (M + H)
1621		465 (M + H)

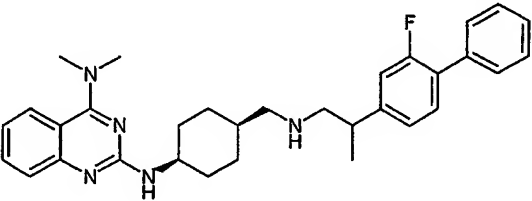
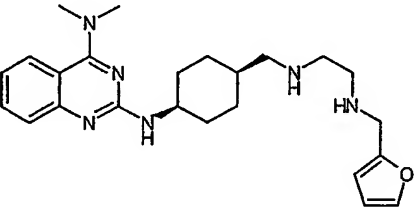
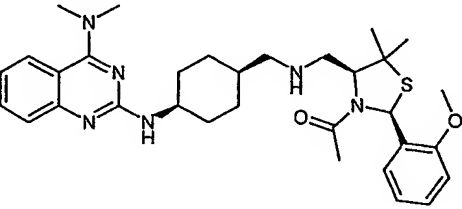
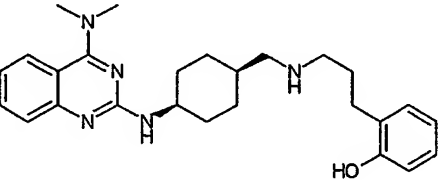
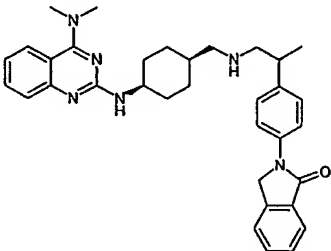
Example No.	Structure	APCI-MS
1622		476 (M + H)
1623		494 (M + H)
1624		453 (M + H)
1625		463 (M + H)
1626		519 (M + H)

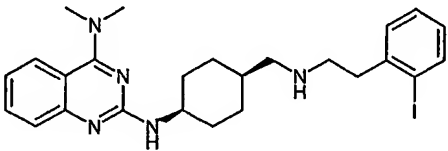
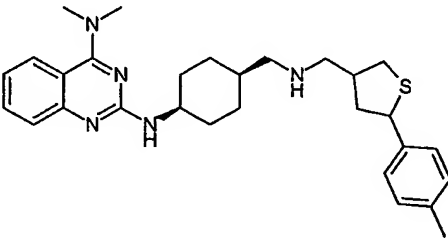
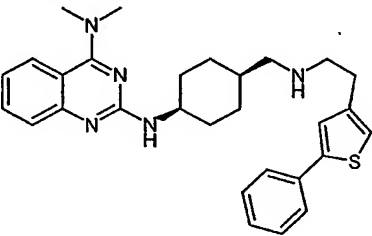
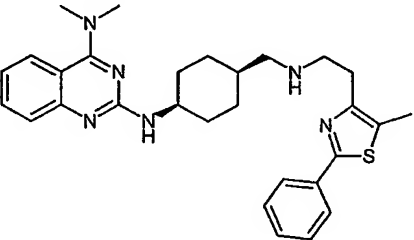
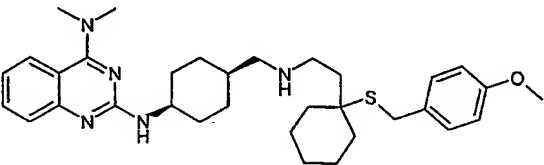
Example No.	Structure	APCI-MS
1627		553 (M + H)
1628		501 (M + H)
1629		458 (M + H)
1630		502 (M + H)
1631		579 (M + H)

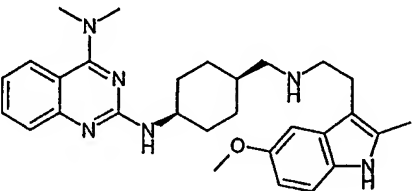
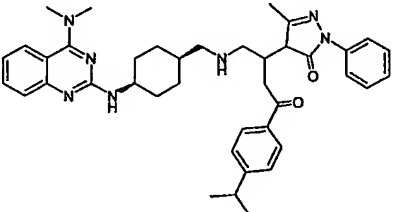
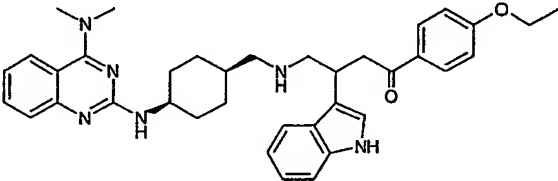
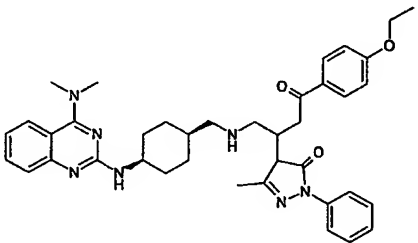
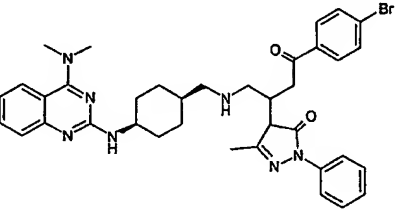
Example No.	Structure	APCI-MS
1632		506 (M + H)
1633		456 (M + H)
1634		530 (M + H)
1635		479 (M + H)
1636		590 (M + H)

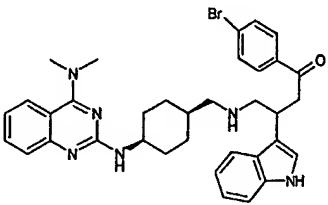
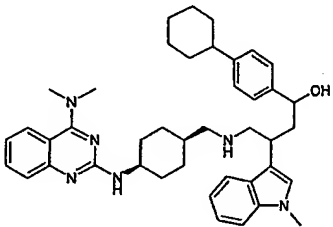
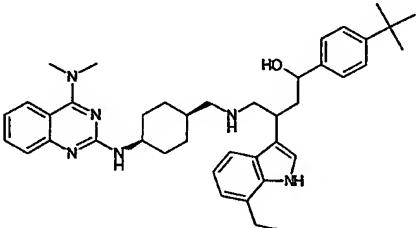
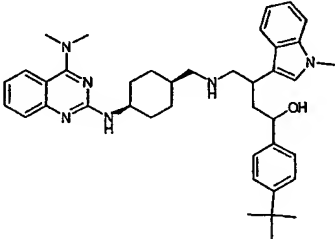
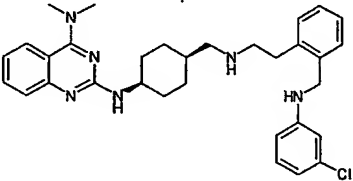
Example No.	Structure	APCI-MS
1637		486 (M + H)
1638		472 (M + H)
1639		480 (M + H)
1640		464 (M + H)
1641		494 (M + H)

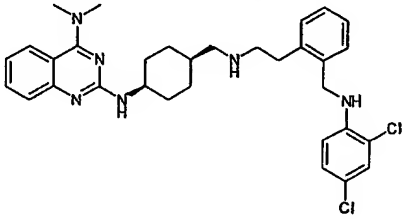
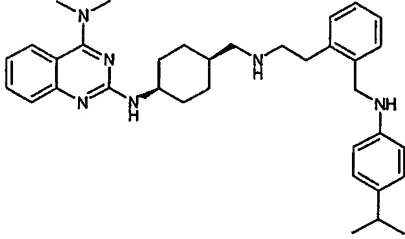
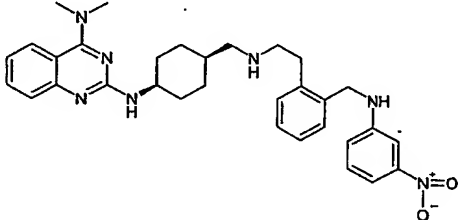
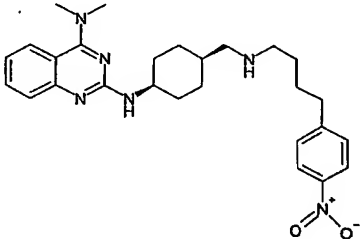
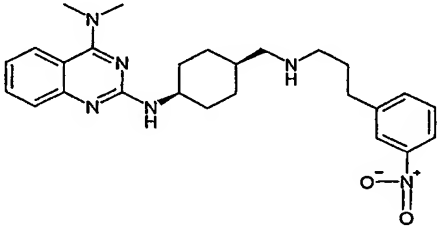
Example No.	Structure	APCI-MS
1642		532 (M + H)
1643		546 (M + H)
1644		608 (M + H)
1645		438 (M + H)
1646		466 (M + H)

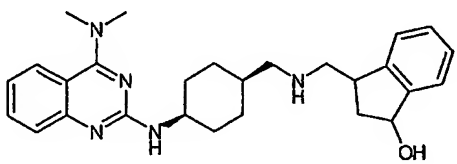
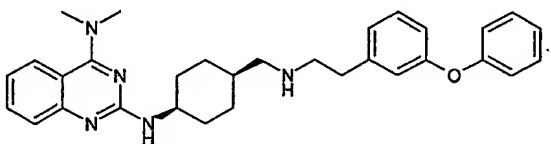
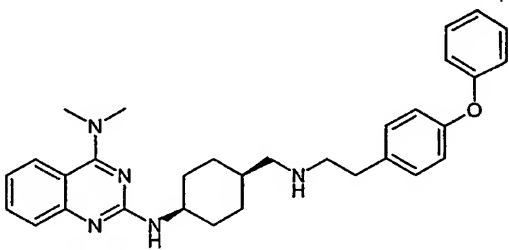
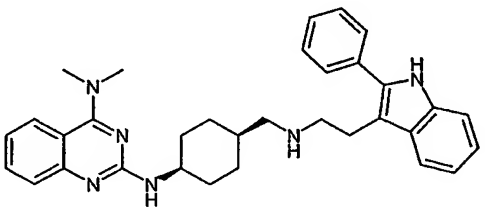
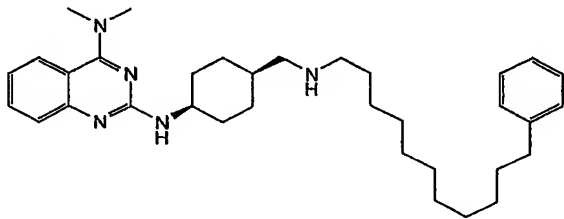
Example No.	Structure	APCI-MS
1647		512 (M + H)
1648		423 (M + H)
1649		577 (M + H)
1650		434 (M + H)
1651		549 (M + H)

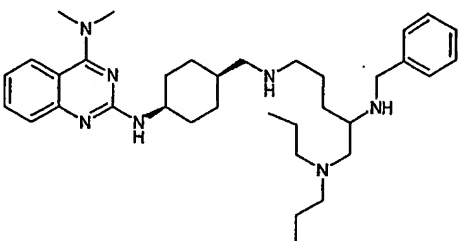
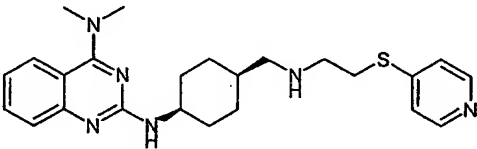
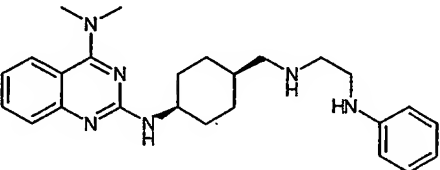
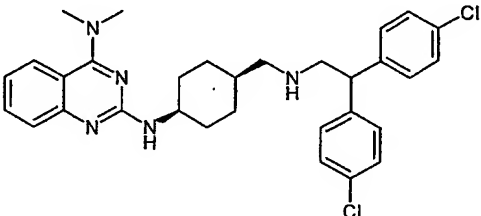
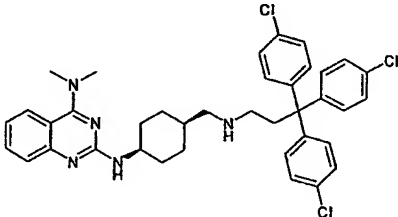
Example No.	Structure	APCI-MS
1652		530 (M + H)
1653		490 (M + H)
1654		486 (M + H)
1655		501 (M + H)
1656		562 (M + H)

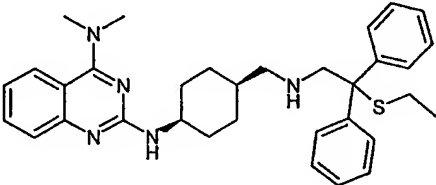
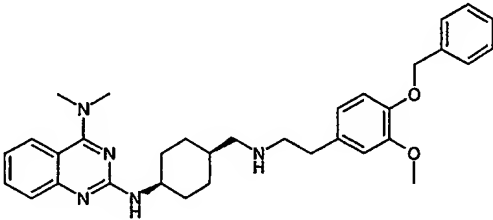
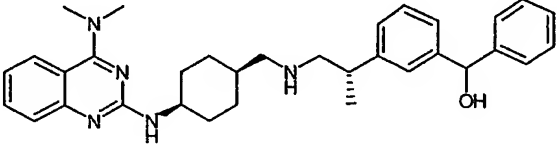
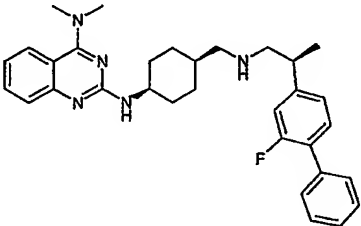
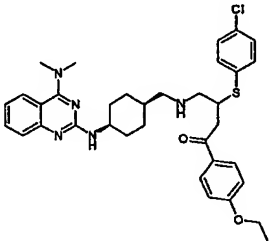
Example No.	Structure	APCI-MS
1657		487 (M + H)
1658		660 (M + H)
1659		605 (M + H)
1660		662 (M + H)
1661		696 (M + H)

Example No.	Structure	APCI-MS
1662		639 (M + H)
1663		659 (M + H)
1664		647 (M + H)
1665		633 (M + H)
1666		543 (M + H)

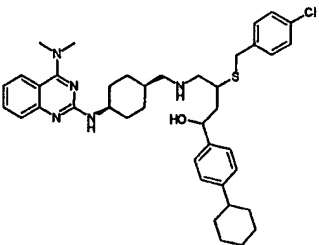
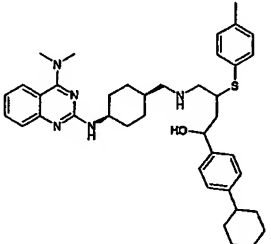
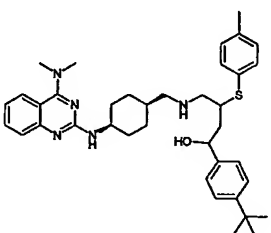
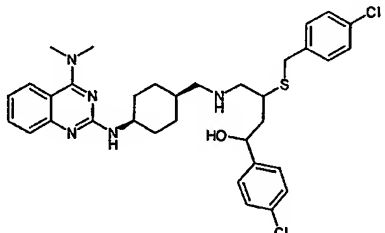
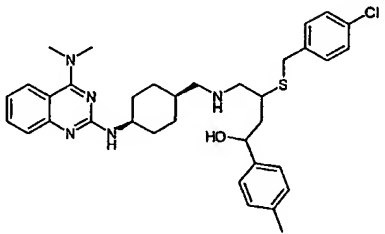
Example No.	Structure	APCI-MS
1667		577 (M + H)
1668		551 (M + H)
1669		554 (M + H)
1670		477 (M + H)
1671		463 (M + H)

Example No.	Structure	APCI-MS
1672		446 (M + H)
1673		496 (M + H)
1674		496 (M + H)
1675		519 (M + H)
1676		530 (M + H)

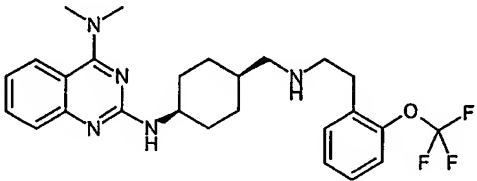
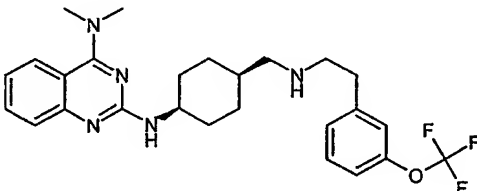
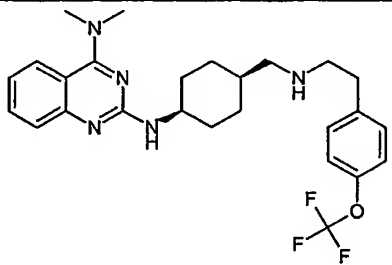
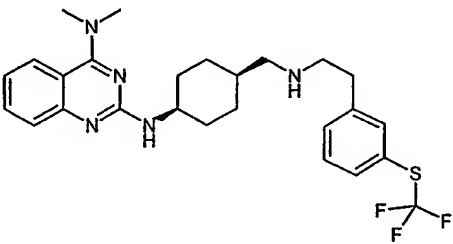
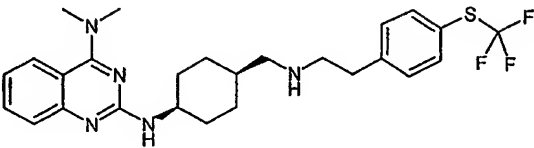
Example No.	Structure	APCI-MS
1677		574 (M + H)
1678		437 (M + H)
1679		419 (M + H)
1680		548 (M + H)
1681		672 (M + H)

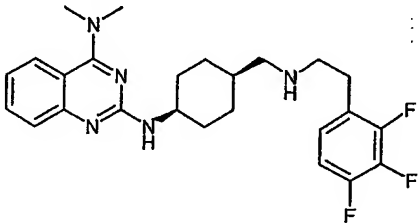
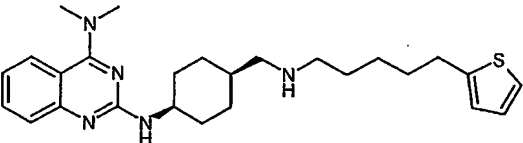
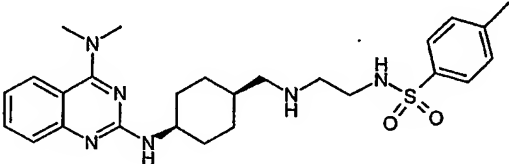
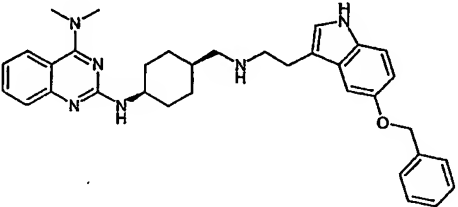
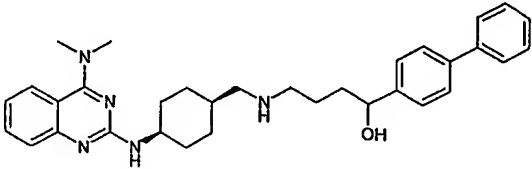
Example No.	Structure	APCI-MS
1682		540 (M + H)
1683		540 (M + H)
1684		524 (M + H)
1685		512 (M + H)
1686		632 (M + H)

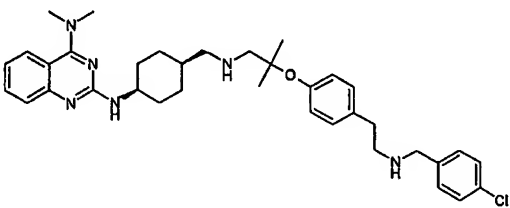
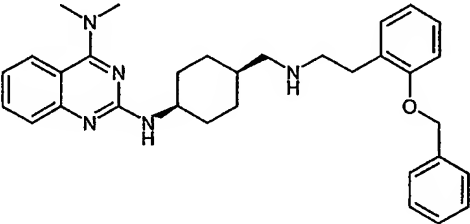
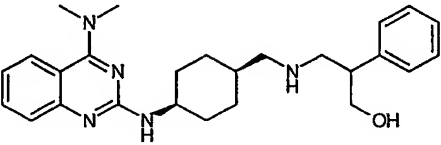
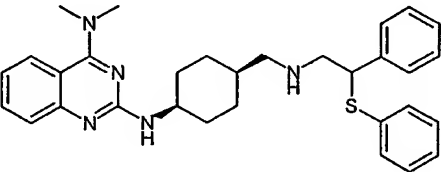
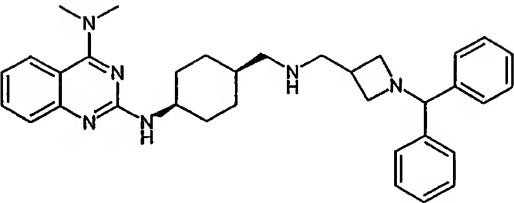
Example No.	Structure	APCI-MS
1687	 <chem>CN1C=NC2=C(N1)C(=NC(=C2)NC3CCCCC3CNC4C(C(C(C4)O)SC5=CC=C(Cl)C=C5)C6=CC=C(C(C)(C)C)C=C6</chem>	646 (M + H)
1688	 <chem>CN1C=NC2=C(N1)C(=NC(=C2)NC3CCCCC3CNC4C(C(C(C4)O)SC5=CC=C(Cl)C=C5)C6=CC=C(OC)C=C6</chem>	648 (M + H)
1689	 <chem>CN1C=NC2=C(N1)C(=NC(=C2)NC3CCCCC3CNC4C(C(C(C4)O)SC5=CC=C(C)C=C5)C6=CC=C(C)C=C6</chem>	584 (M + H)
1690	 <chem>CN1C=NC2=C(N1)C(=NC(=C2)NC3CCCCC3CNC4C(C(C(C4)O)SC5=CC=C(Cl)C=C5)C6=CC=C(C(C)C)C=C6</chem>	632 (M + H)
1691	 <chem>CN1C=NC2=C(N1)C(=NC(=C2)NC3CCCCC3CNC4C(C(C(C4)O)SC5=CC=C(Cl)C=C5)C6=CC=C(C7CCCCC7)C=C6</chem>	672 (M + H)

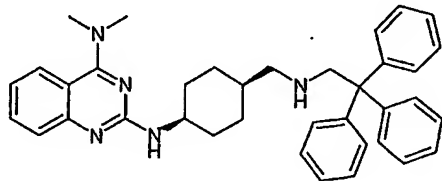
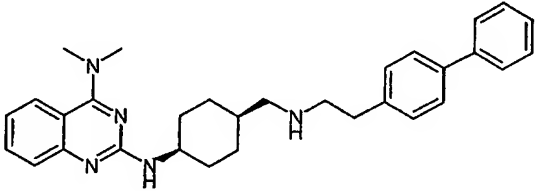
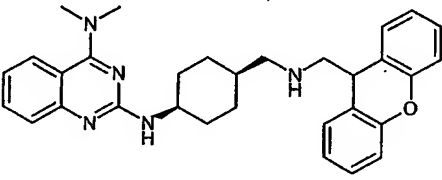
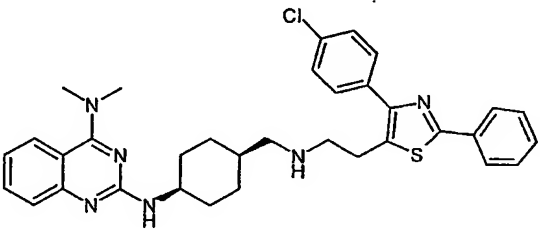
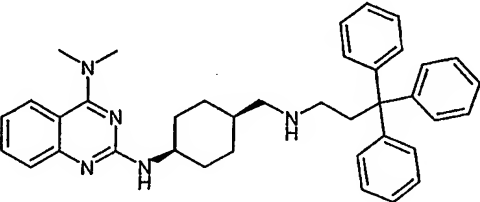
Example No.	Structure	APCI-MS
1692		686 (M + H)
1693		652 (M + H)
1694		626 (M + H)
1695		638 (M + H)
1696		618 (M + H)

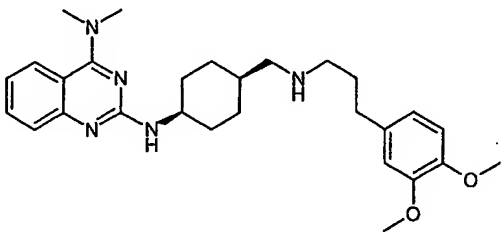
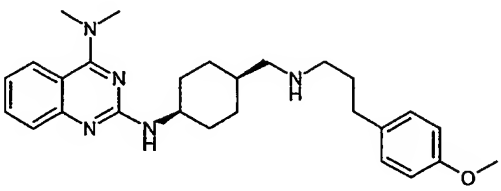
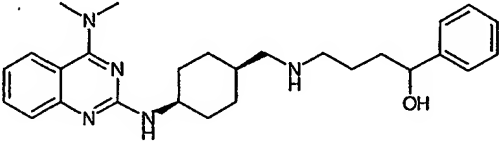
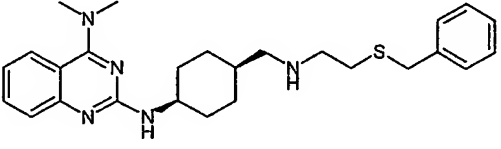
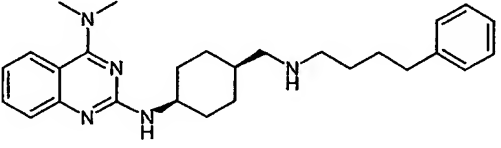
Example No.	Structure	APCI-MS
1697		612 (M + H)
1698		588 (M + H)
1699		624 (M + H)
1700		438 (M + H)
1701		522 (M + H)

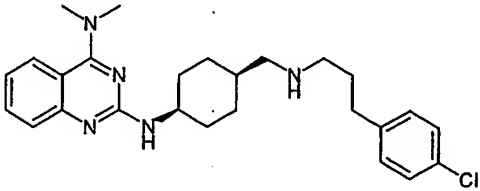
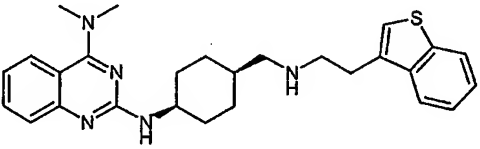
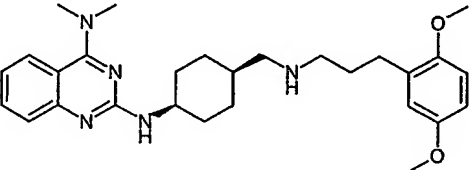
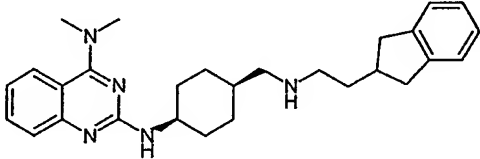
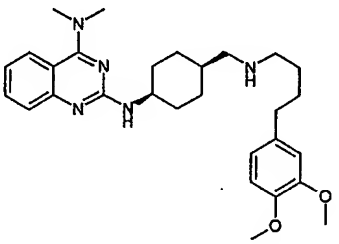
Example No.	Structure	APCI-MS
1702		488 (M + H)
1703		488 (M + H)
1704		488 (M + H)
1705		504 (M + H)
1706		504 (M + H)

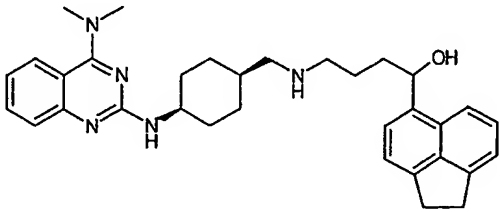
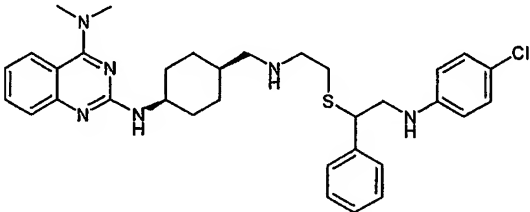
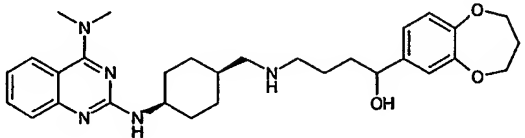
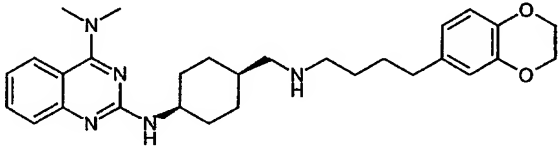
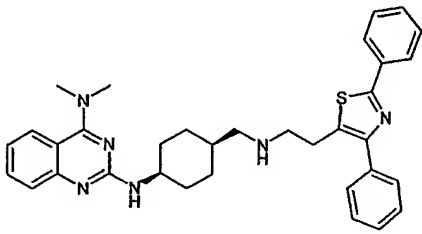
Example No.	Structure	APCI-MS
1707		458 (M + H)
1708		452 (M + H)
1709		497 (M + H)
1710		549 (M + H)
1711		524 (M + H)

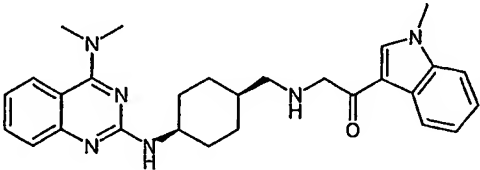
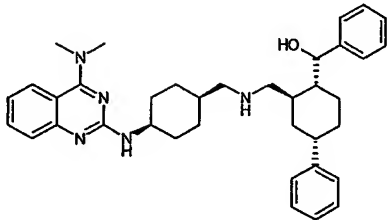
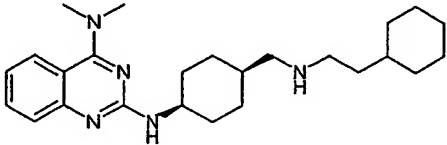
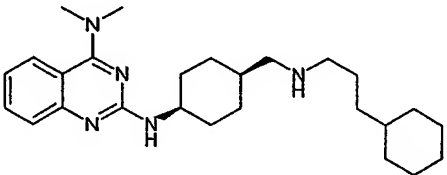
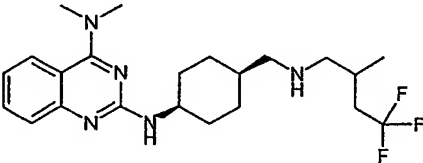
Example No.	Structure	APCI-MS
1712		615 (M + H)
1713		510 (M + H)
1714		434 (M + H)
1715		512 (M + H)
1716		535 (M + H)

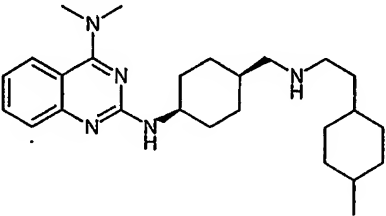
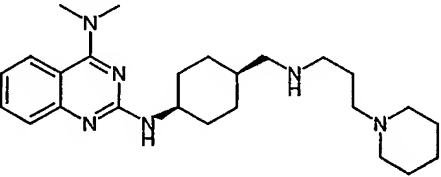
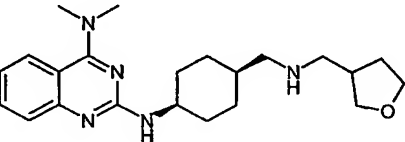
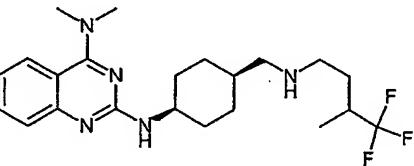
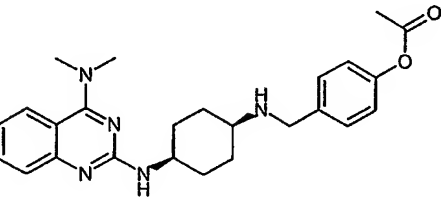
Example No.	Structure	APCI-MS
1717		556 (M + H)
1718		480 (M + H)
1719		494 (M + H)
1720		597 (M + H)
1721		570 (M + H)

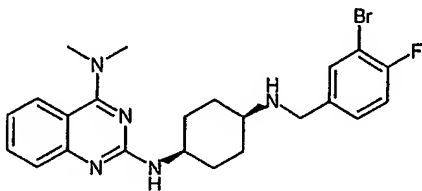
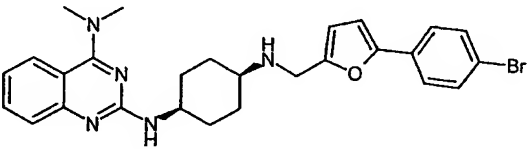
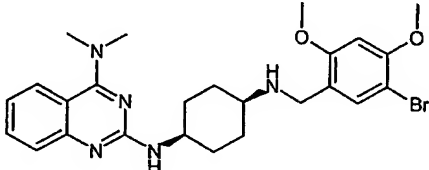
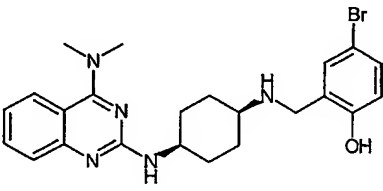
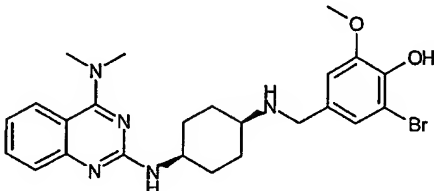
Example No.	Structure	APCI-MS
1722		478 (M + H)
1723		448 (M + H)
1724		448 (M + H)
1725		450 (M + H)
1726		432 (M + H)

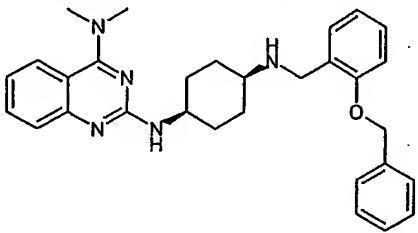
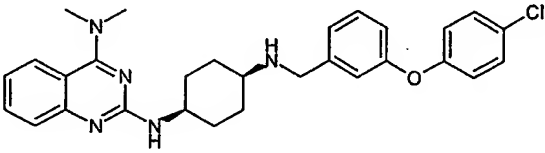
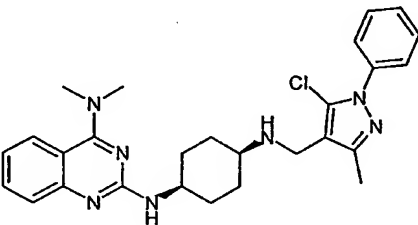
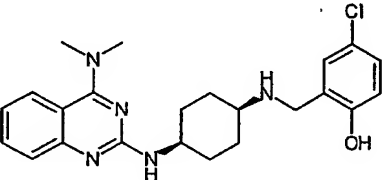
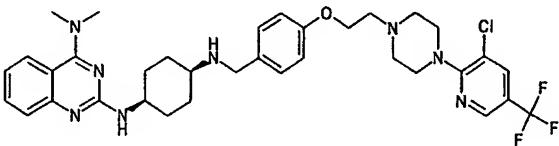
Example No.	Structure	APCI-MS
1727		452 (M + H)
1728		460 (M + H)
1729		478 (M + H)
1730		444 (M + H)
1731		492 (M + H)

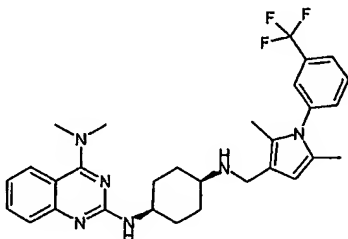
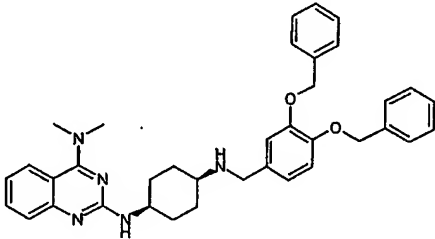
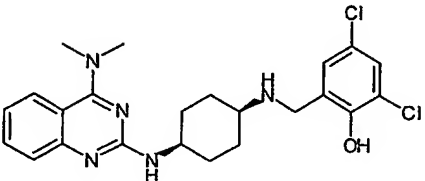
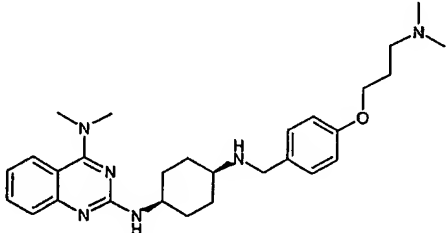
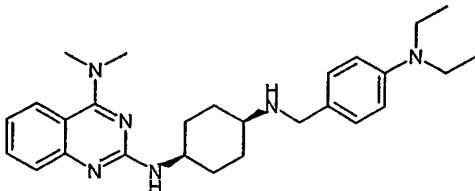
Example No.	Structure	APCI-MS
1732		524 (M + H)
1733		589 (M + H)
1734		520 (M + H)
1735		490 (M + H)
1736		563 (M + H)

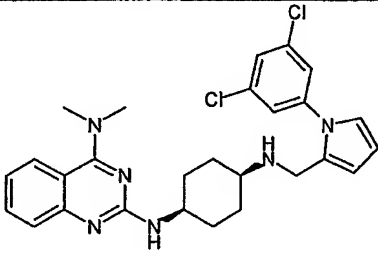
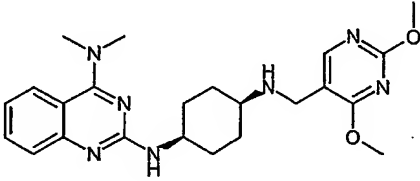
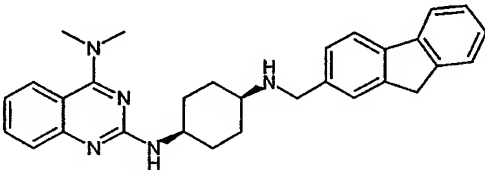
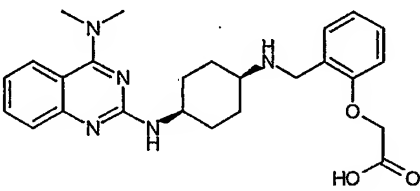
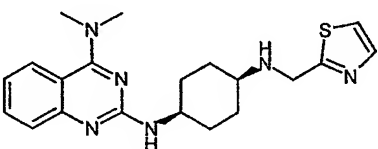
Example No.	Structure	APCI-MS
1737		471 (M + H)
1738		578 (M + H)
1739		410 (M + H)
1740		424 (M + H)
1741		424 (M + H)

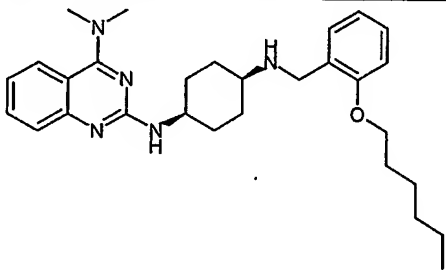
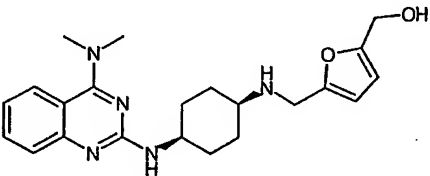
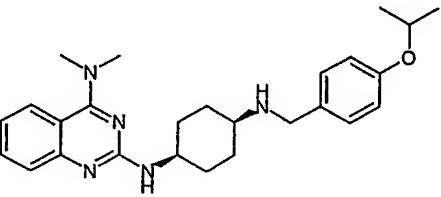
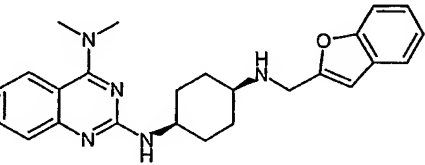
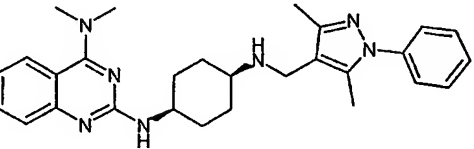
Example No.	Structure	APCI-MS
1742		424 (M + H)
1743		447 (M + Na)
1744		384 (M + H)
1745		424 (M + H)
1746		434 (M + H)

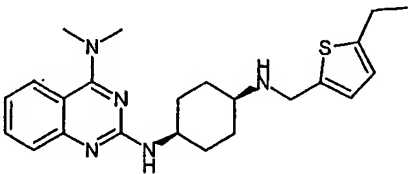
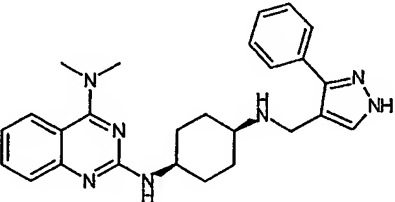
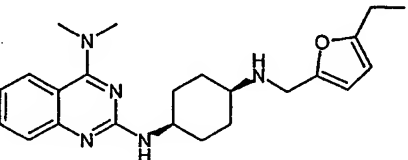
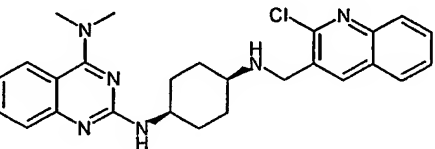
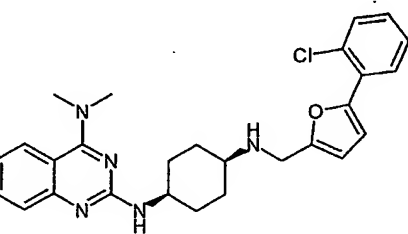
Example No.	Structure	APCI-MS
1747		472 (M + H)
1748		520 (M + H)
1749		514 (M + H)
1750		470 (M + H)
1751		500 (M + H)

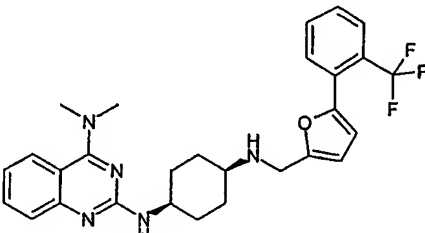
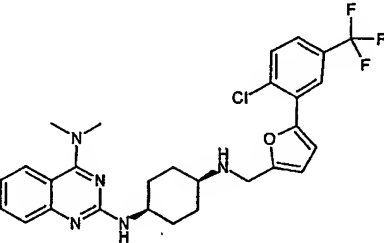
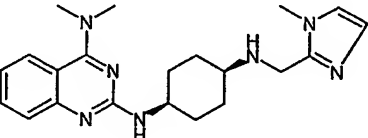
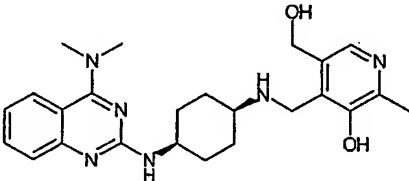
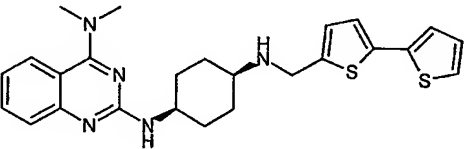
Example No.	Structure	APCI-MS
1752		482 (M + H)
1753		502 (M + H)
1754		490 (M + H)
1755		426 (M + H)
1756		683 (M + H)

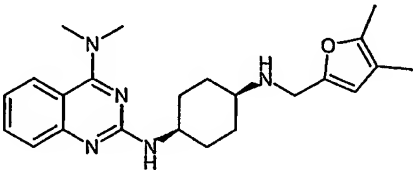
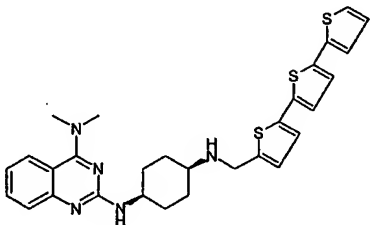
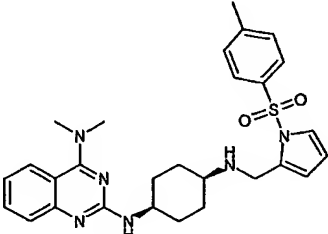
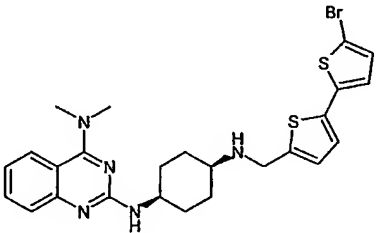
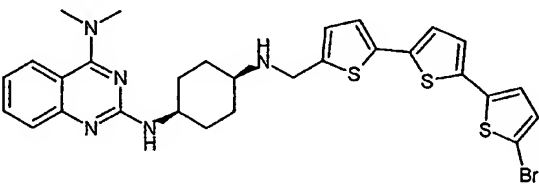
Example No.	Structure	APCI-MS
1757		537 (M + H)
1758		588 (M + H)
1759		460 (M + H)
1760		477 (M + H)
1761		447 (M + H)

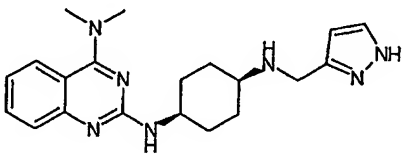
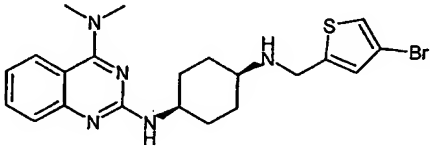
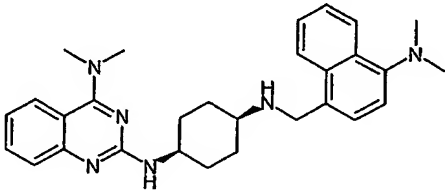
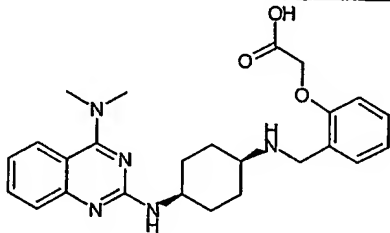
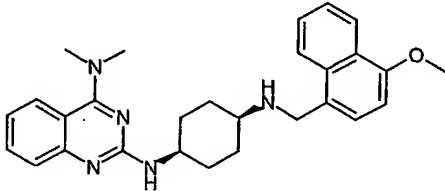
Example No.	Structure	APCI-MS
1762		509 (M + H)
1763		438 (M + H)
1764		464 (M + H)
1765		450 (M + H)
1766		383 (M + H)

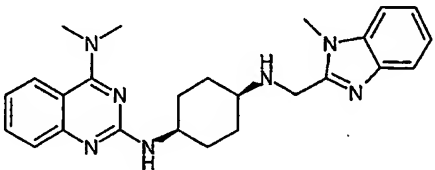
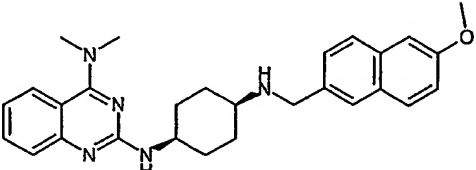
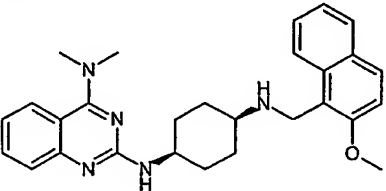
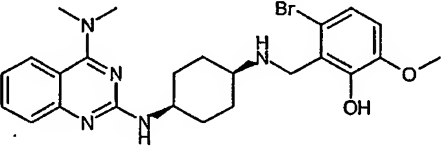
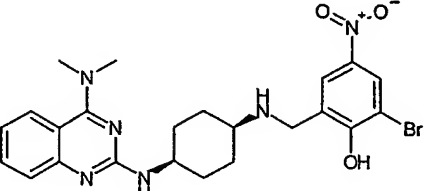
Example No.	Structure	APCI-MS
1767		476 (M + H)
1768		396 (M + H)
1769		434 (M + H)
1770		416 (M + H)
1771		470 (M + H)

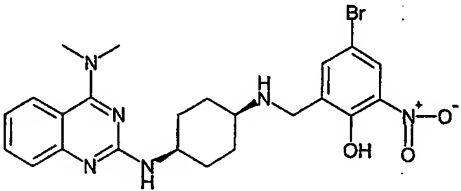
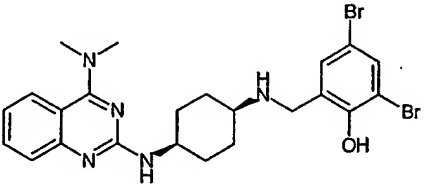
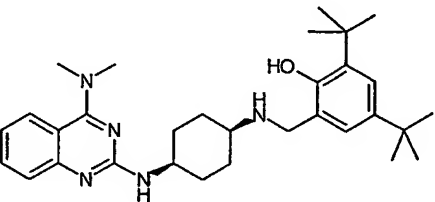
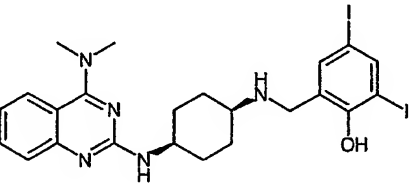
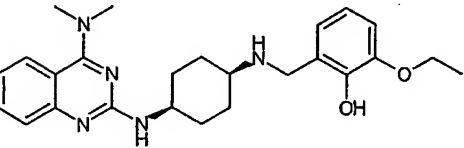
Example No.	Structure	APCI-MS
1772		410 (M + H)
1773		442 (M + H)
1774		394 (M + H)
1775		461 (M + H)
1776		476 (M + H)

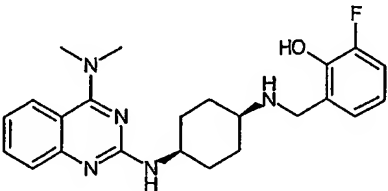
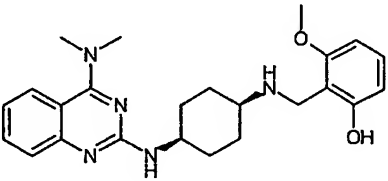
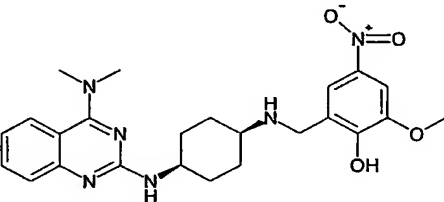
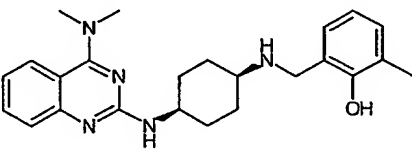
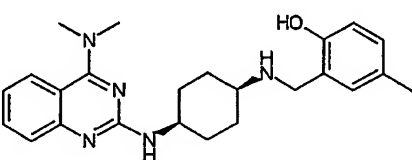
Example No.	Structure	APCI-MS
1777		510 (M + H)
1778		544 (M + H)
1779		380 (M + H)
1780		437 (M + H)
1781		464 (M + H)

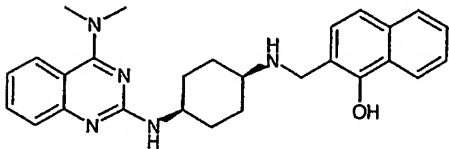
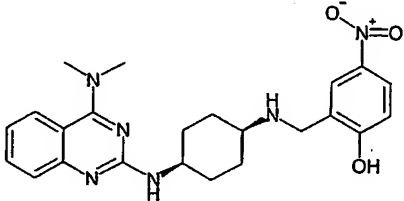
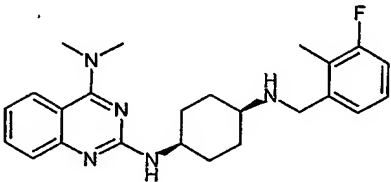
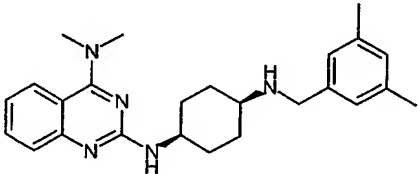
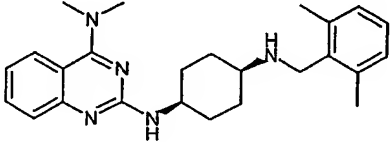
Example No.	Structure	APCI-MS
1782		394 (M + H)
1783		546 (M + H)
1784		519 (M + H)
1785		542 (M + H)
1786		624 (M + H)

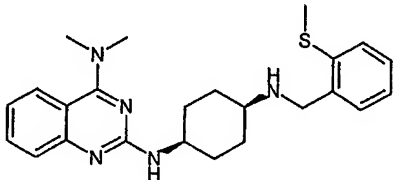
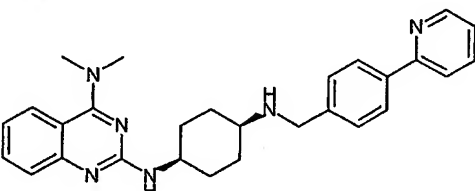
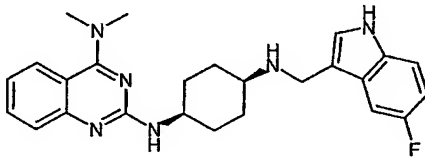
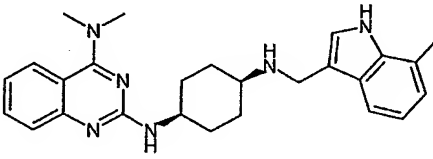
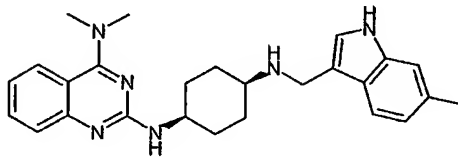
Example No.	Structure	APCI-MS
1787		366 (M + H)
1788		460 (M + H)
1789		469 (M + H)
1790		450 (M + H)
1791		456 (M + H)

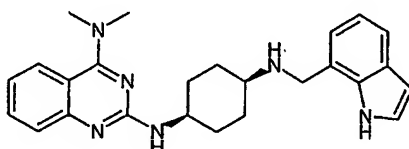
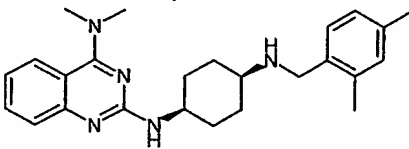
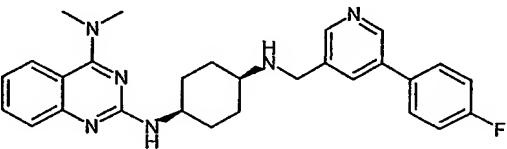
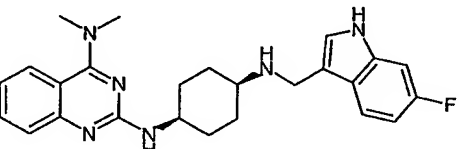
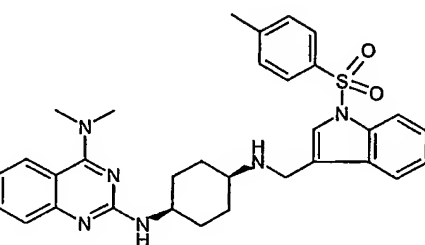
Example No.	Structure	APCI-MS
1792		430 (M + H)
1793		456 (M + H)
1794		456 (M + H)
1795		500 (M + H)
1796		537 (M + Na)

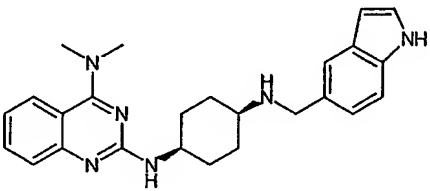
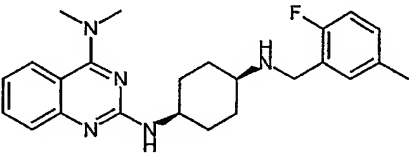
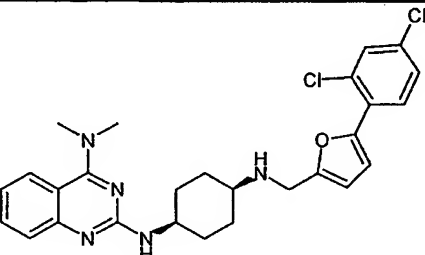
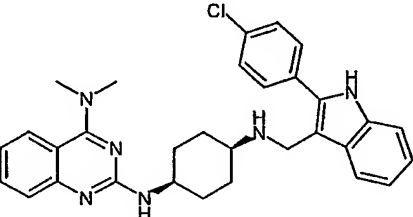
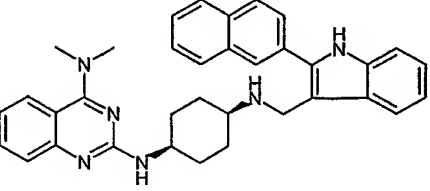
Example No.	Structure	APCI-MS
1797		537 (M + Na)
1798		548 (M + H)
1799		504 (M + H)
1800		644 (M + H)
1801		436 (M + H)

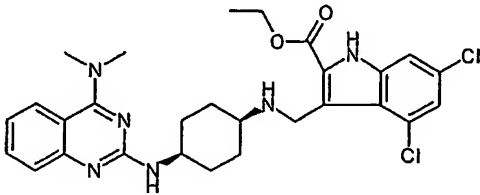
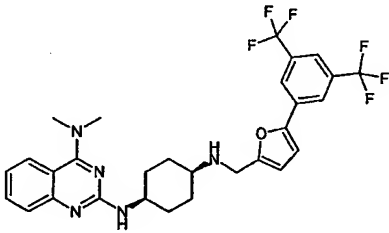
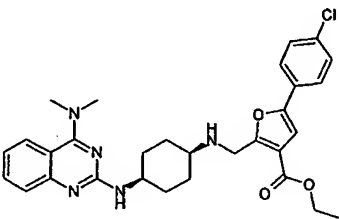
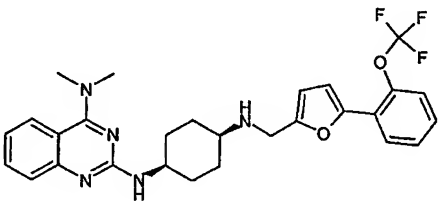
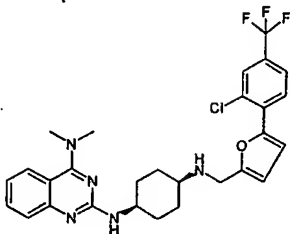
Example No.	Structure	APCI-MS
1802		410 (M + H)
1803		422 (M + H)
1804		467 (M + H)
1805		406 (M + H)
1806		406 (M + H)

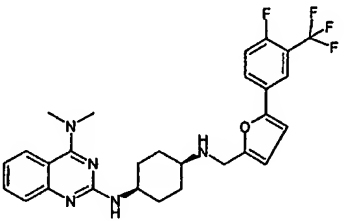
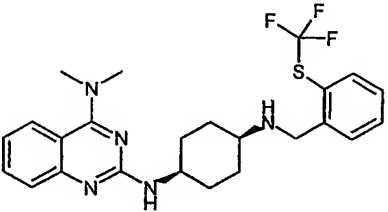
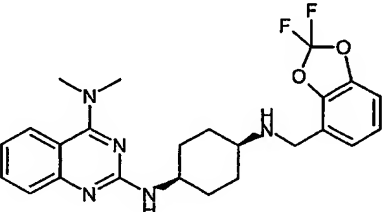
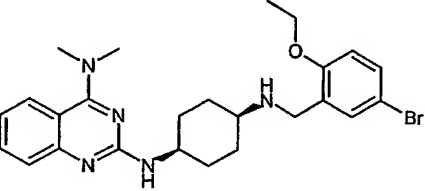
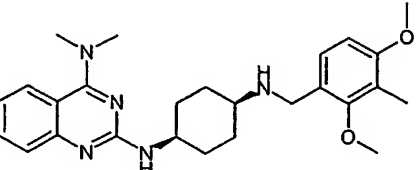
Example No.	Structure	APCI-MS
1807		440 (M - H)
1808		437 (M + H)
1809		408 (M + H)
1810		404 (M + H)
1811		404 (M + H)

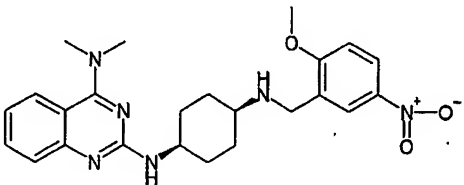
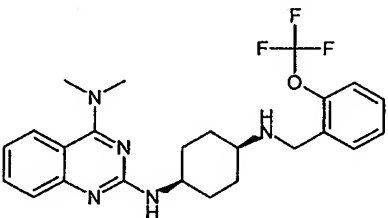
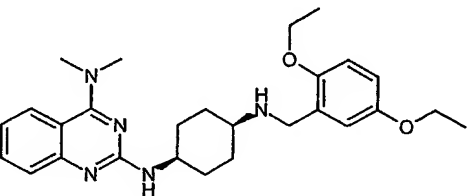
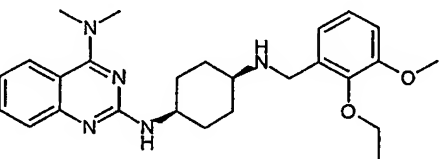
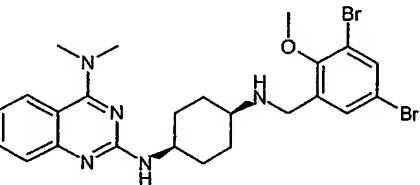
Example No.	Structure	APCI-MS
1812		422 (M + H)
1813		453 (M + H)
1814		433 (M + H)
1815		429 (M + H)
1816		429 (M + H)

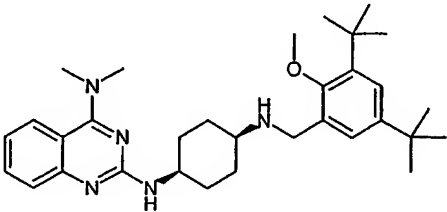
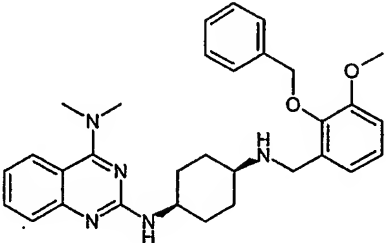
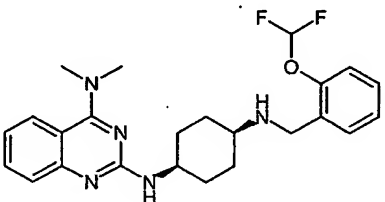
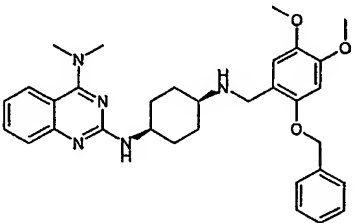
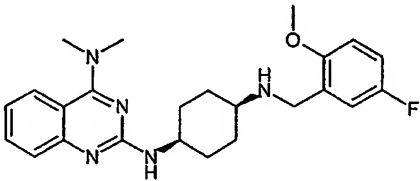
Example No.	Structure	APCI-MS
1817		415 (M + H)
1818		404 (M + H)
1819		471 (M + H)
1820		433 (M + H)
1821		569 (M + H)

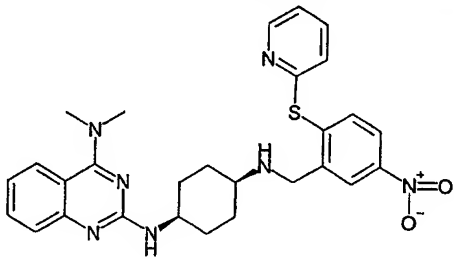
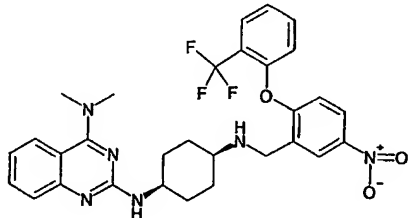
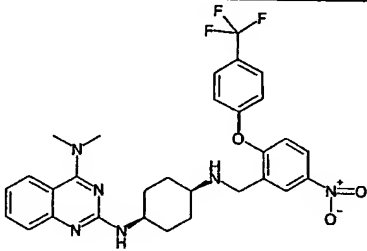
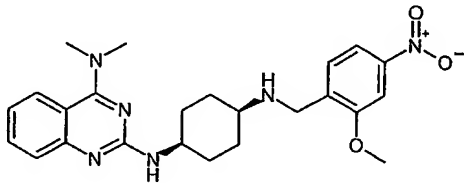
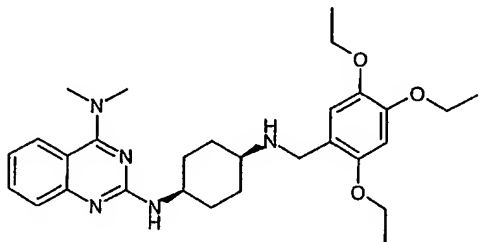
Example No.	Structure	APCI-MS
1822		415 (M + H)
1823		408 (M + H)
1824		510 (M + H)
1825		525 (M + H)
1826		541 (M + H)

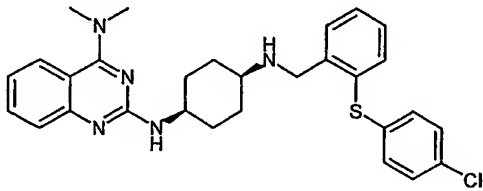
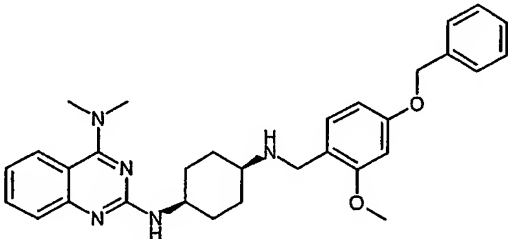
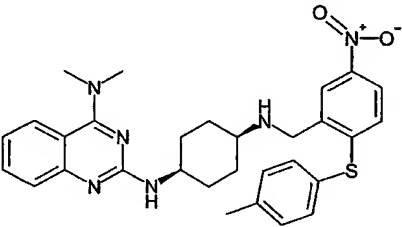
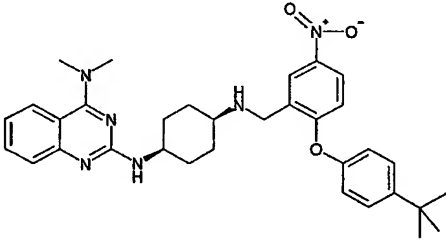
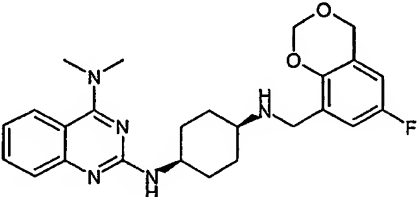
Example No.	Structure	APCI-MS
1827		555 (M + H)
1828		578 (M + H)
1829		548 (M + H)
1830		526 (M + H)
1831		544 (M + H)

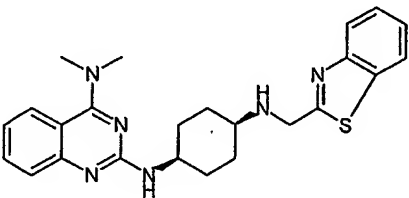
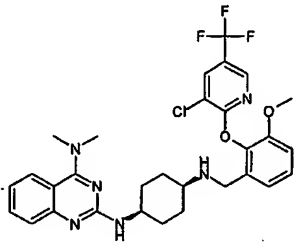
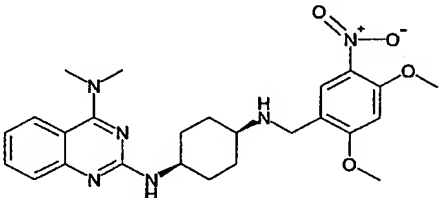
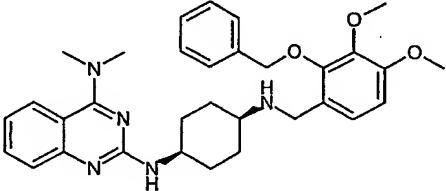
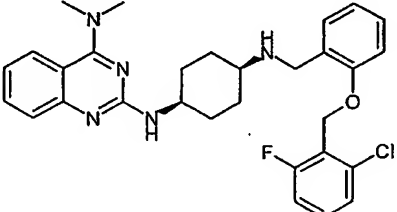
Example No.	Structure	APCI-MS
1832		528 (M + H)
1833		476 (M + H)
1834		456 (M + H)
1835		498 (M + H)
1836		450 (M + H)

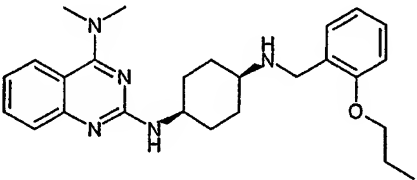
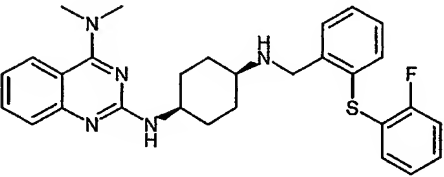
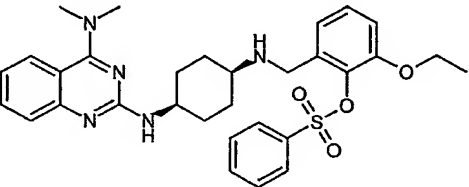
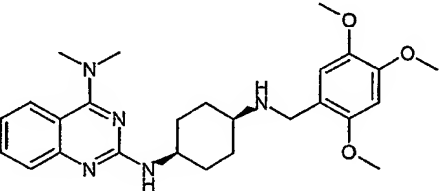
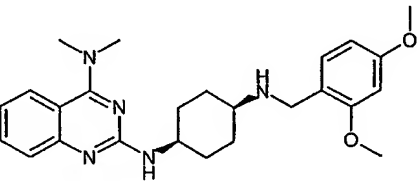
Example No.	Structure	APCI-MS
1837		451 (M + H)
1838		460 (M + H)
1839		464 (M + H)
1840		450 (M + H)
1841		562 (M + H)

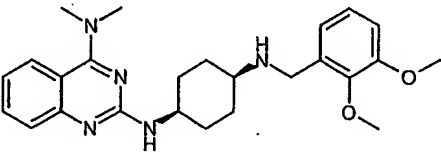
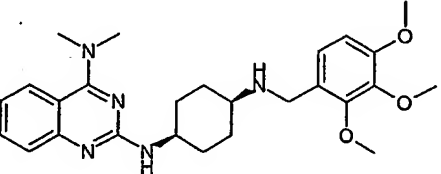
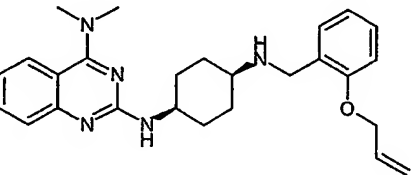
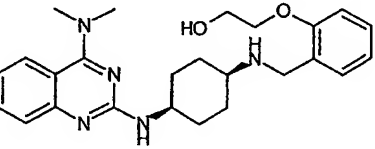
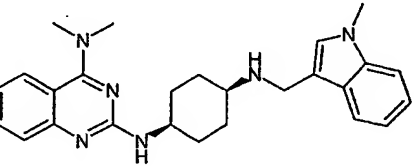
Example No.	Structure	APCI-MS
1842		518 (M + H)
1843		512 (M + H)
1844		442 (M + H)
1845		542 (M + H)
1846		424 (M + H)

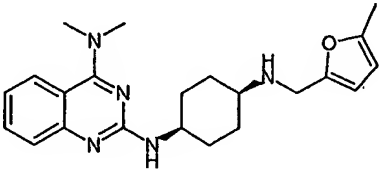
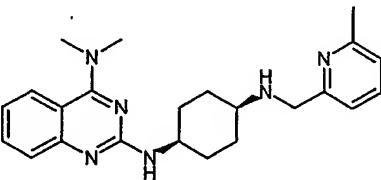
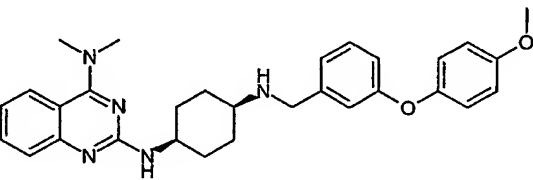
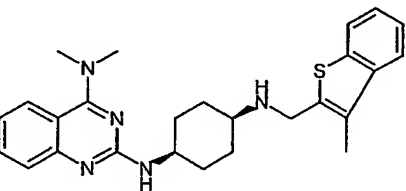
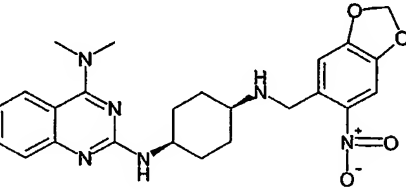
Example No.	Structure	APCI-MS
1847		530 (M + H)
1848		581 (M + H)
1849		581 (M + H)
1850		451 (M + H)
1851		508 (M + H)

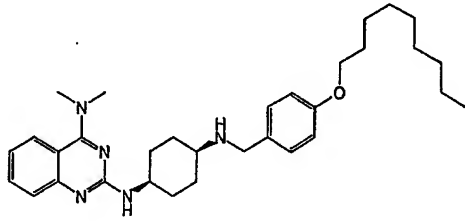
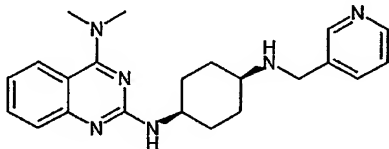
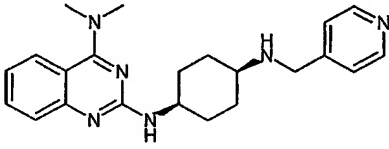
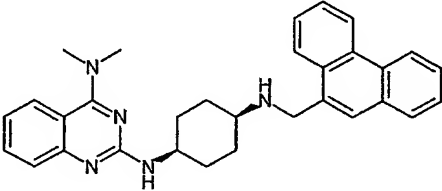
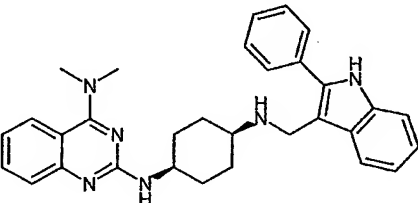
Example No.	Structure	APCI-MS
1852		518 (M + H)
1853		512 (M + H)
1854		543 (M + H)
1855		569 (M + H)
1856		452 (M + H)

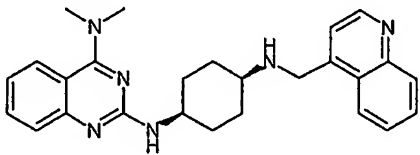
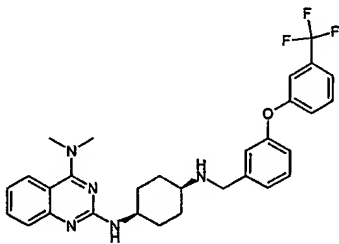
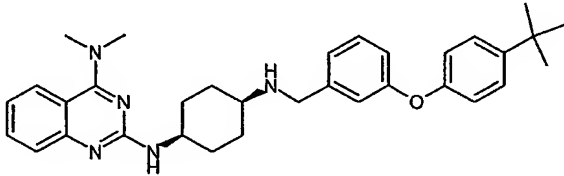
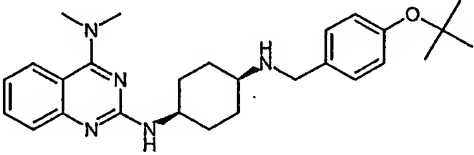
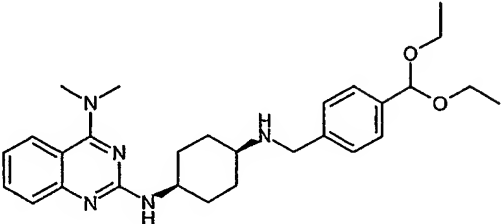
Example No.	Structure	APCI-MS
1857		433 (M + H)
1858		601 (M + H)
1859		481 (M + H)
1860		542 (M + H)
1861		534 (M + H)

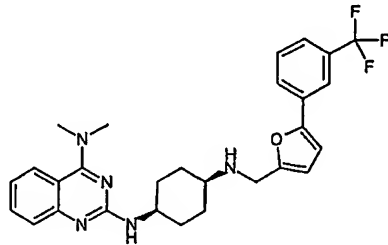
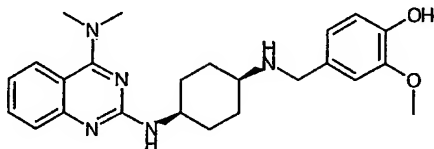
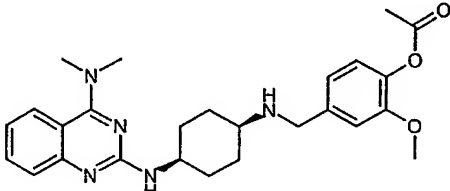
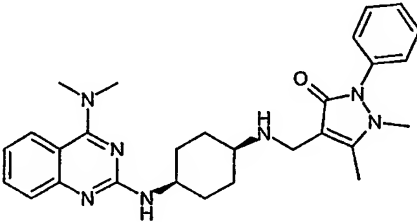
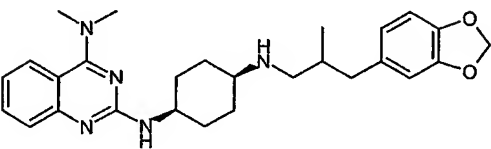
Example No.	Structure	APCI-MS
1862		434 (M + H)
1863		502 (M + H)
1864		576 (M + H)
1865		466 (M + H)
1866		436 (M + H)

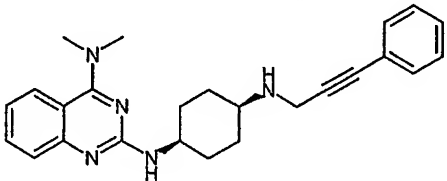
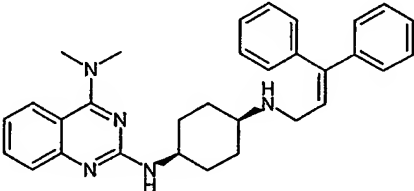
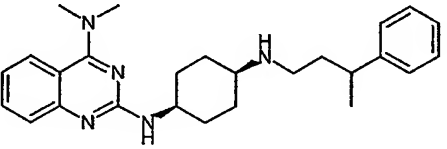
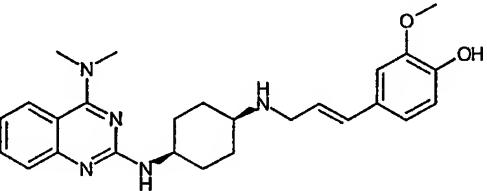
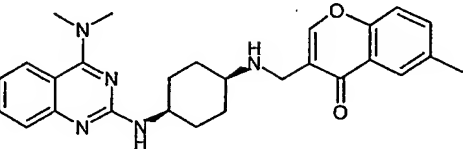
Example No.	Structure	APCI-MS
1867		436 (M + H)
1868		466 (M + H)
1869		432 (M + H)
1870		436 (M + H)
1871		429 (M + H)

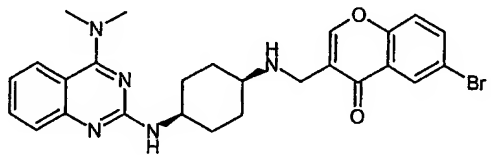
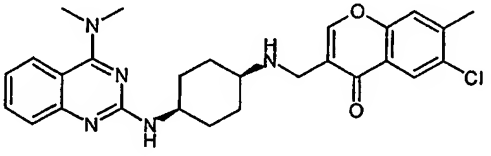
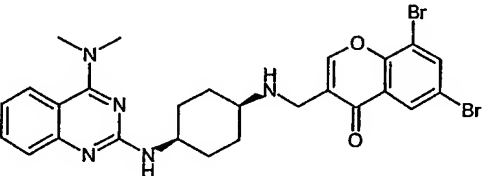
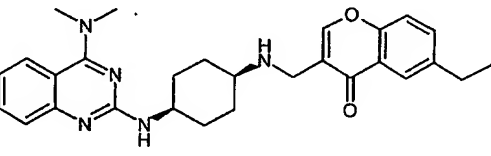
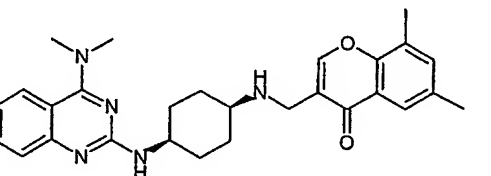
Example No.	Structure	APCI-MS
1872		380 (M + H)
1873		391 (M + H)
1874		498 (M + H)
1875		446 (M + H)
1876		465 (M + H)

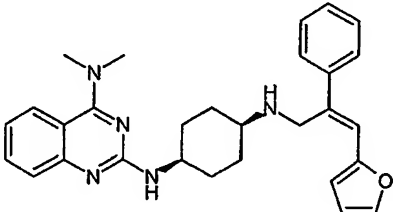
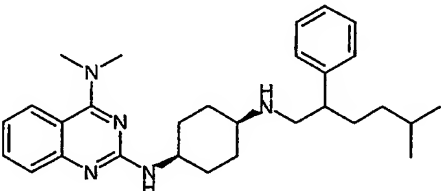
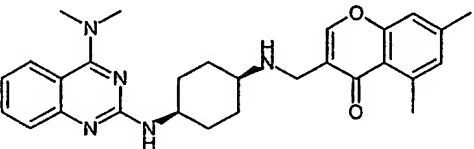
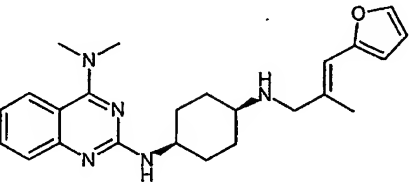
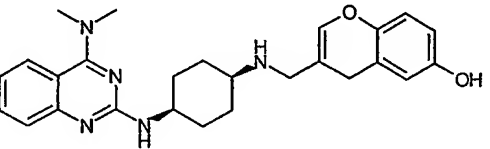
Example No.	Structure	APCI-MS
1877		518 (M + H)
1878		377 (M + H)
1879		377 (M + H)
1880		476 (M + H)
1881		491 (M + H)

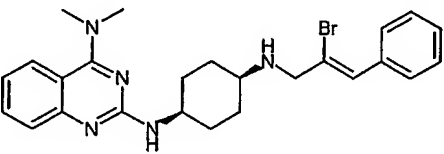
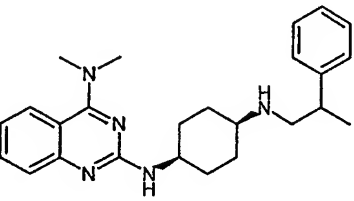
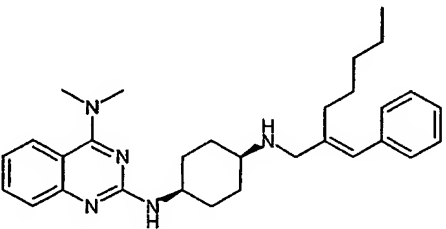
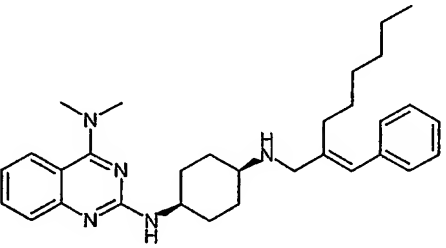
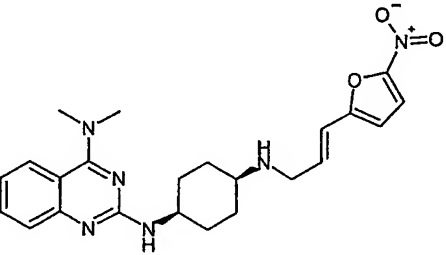
Example.No.	Structure	APCI-MS
1882		427 (M + H)
1883		536 (M + H)
1884		524 (M + H)
1885		448 (M + H)
1886		478 (M + H)

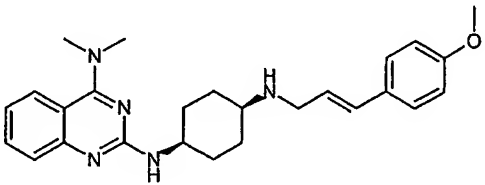
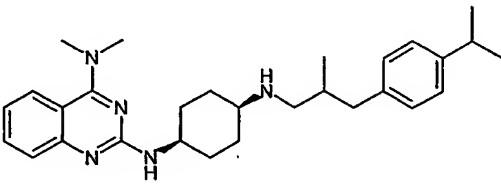
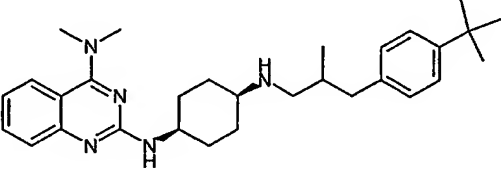
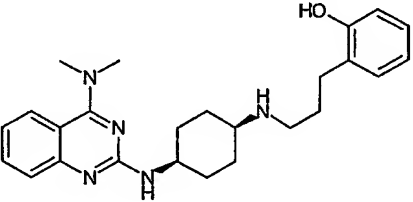
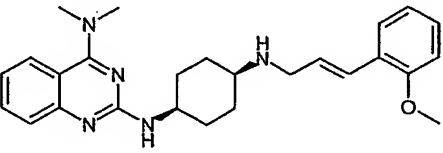
Example No.	Structure	APCI-MS
1887		510 (M + H)
1888		422 (M + H)
1889		464 (M + H)
1890		486 (M + H)
1891		462 (M + H)

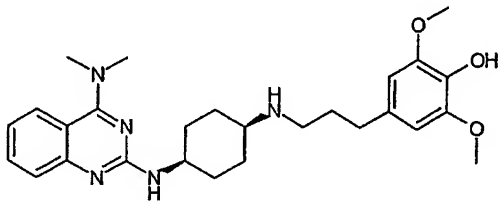
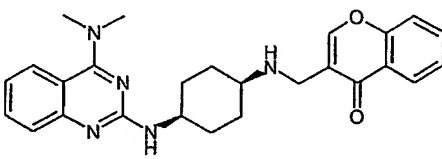
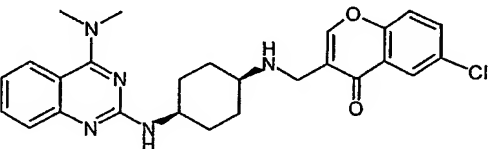
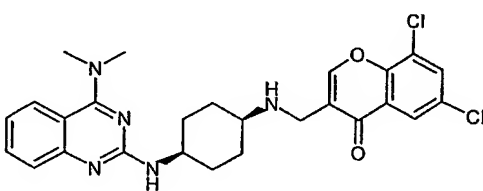
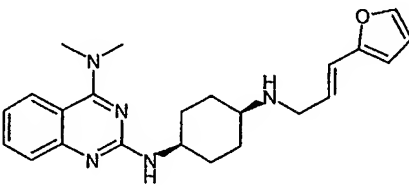
Example No.	Structure	APCI-MS
1892		400 (M + H)
1893		478 (M + H)
1894		418 (M + H)
1895		448 (M + H)
1896		458 (M + H)

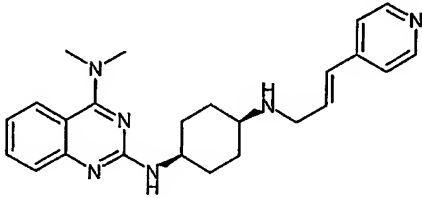
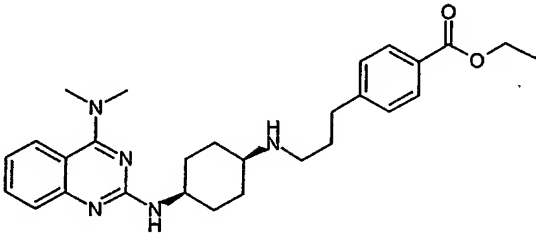
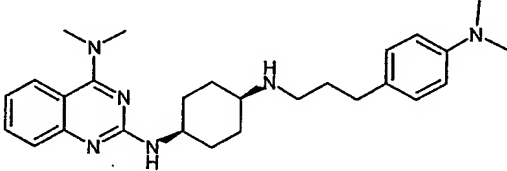
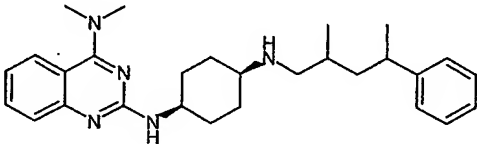
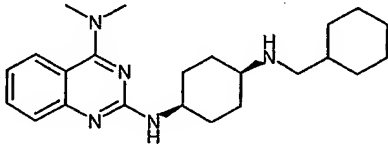
Example No.	Structure	APCI-MS
1897		522 (M + H)
1898		492 (M + H)
1899		600 (M + H)
1900		472 (M + H)
1901		472 (M + H)

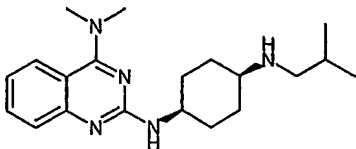
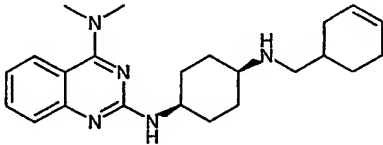
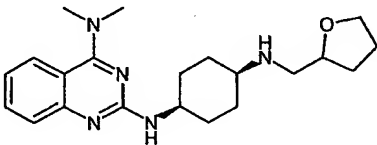
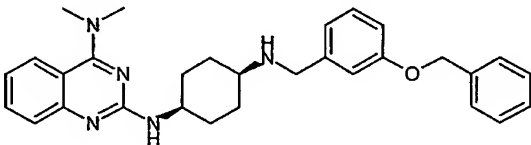
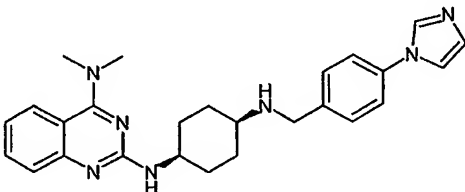
Example No.	Structure	APCI-MS
1902		468 (M + H)
1903		460 (M + H)
1904		472 (M + H)
1905		406 (M + H)
1906		446 (M + H)

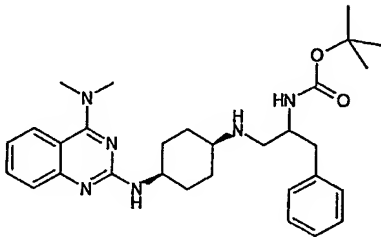
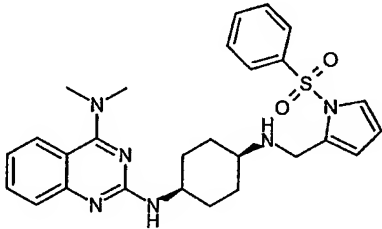
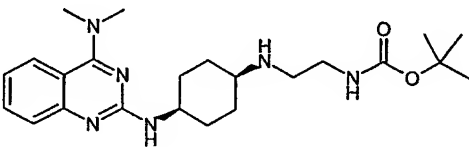
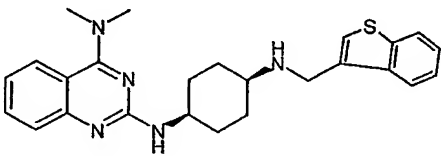
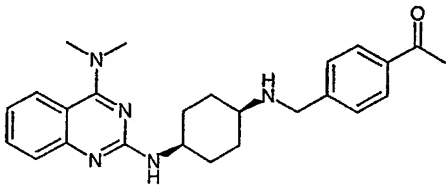
Example No.	Structure	APCI-MS
1907		480 (M + H)
1908		404 (M + H)
1909		472 (M + H)
1910		486 (M + H)
1911		437 (M + H)

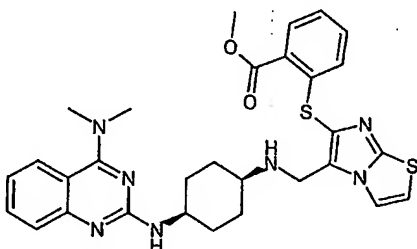
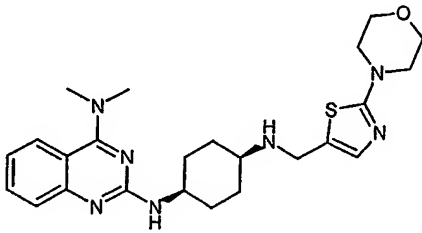
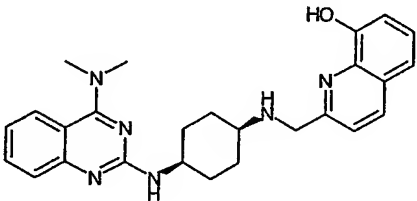
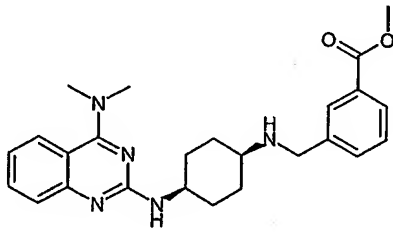
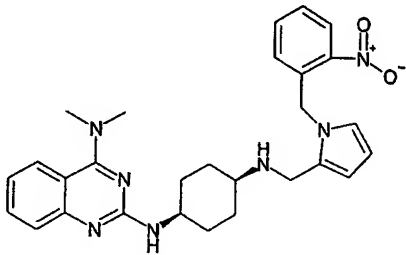
Example No.	Structure	APCI-MS
1912		432 (M + H)
1913		460 (M + H)
1914		474 (M + H)
1915		420 (M + H)
1916		432 (M + H)

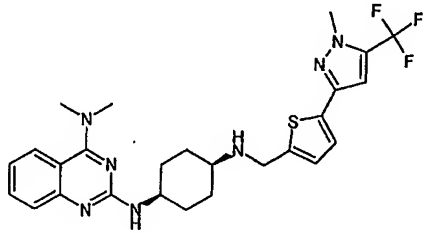
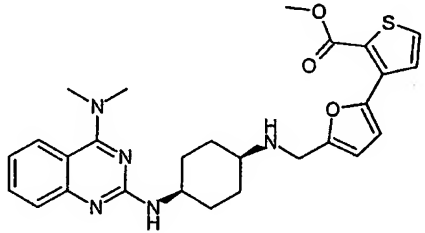
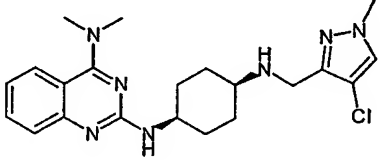
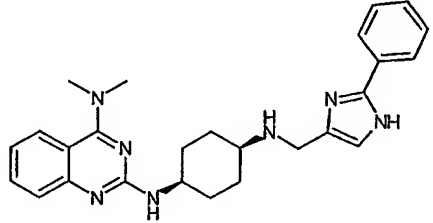
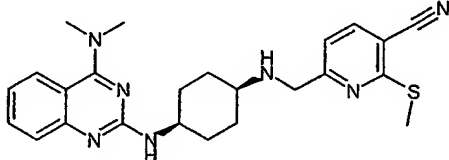
Example No.	Structure	APCI-MS
1917		480 (M + H)
1918		444 (M + H)
1919		478 (M + H)
1920		512 (M + H)
1921		392 (M + H)

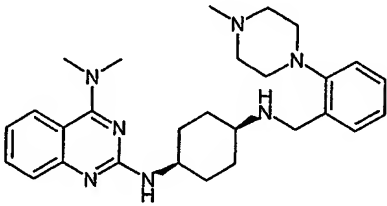
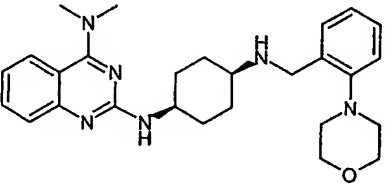
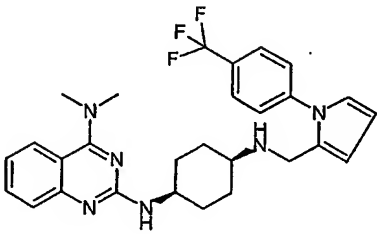
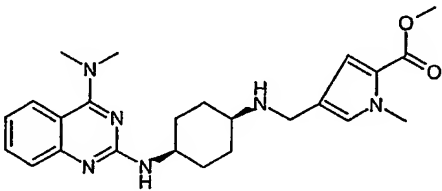
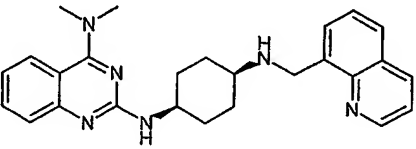
Example No.	Structure	APCI-MS
1922		403 (M + H)
1923		476 (M + H)
1924		447 (M + H)
1925		446 (M + H)
1926		382 (M + H)

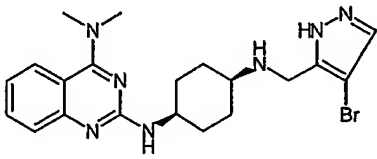
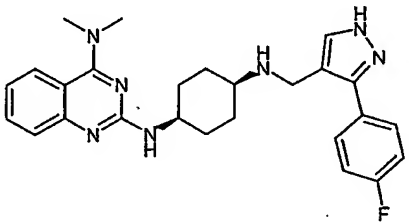
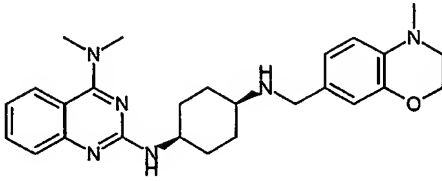
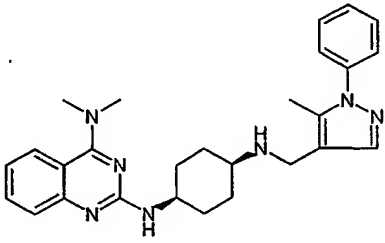
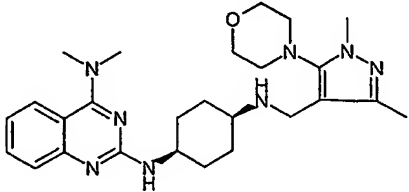
Example No.	Structure	APCI-MS
1927		342 (M + H)
1928		380 (M + H)
1929		370 (M + H)
1930		482 (M + H)
1931		442 (M + H)

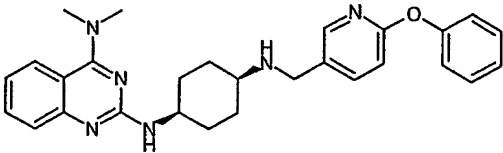
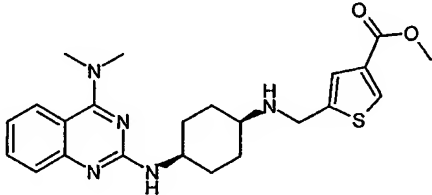
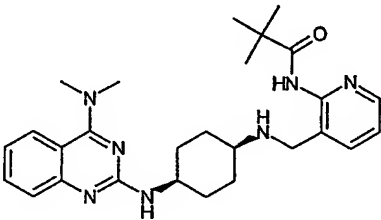
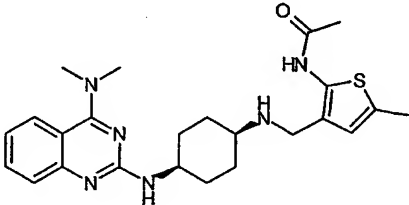
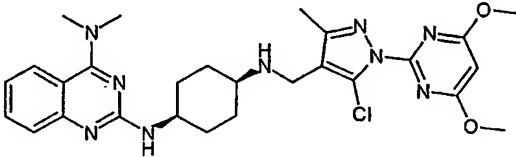
Example No.	Structure	APCI-MS
1932		519 (M + H)
1933		505 (M + H)
1934		429 (M + H)
1935		432 (M + H)
1936		418 (M + H)

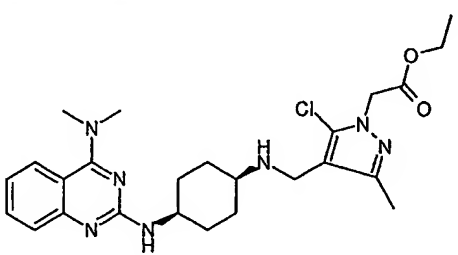
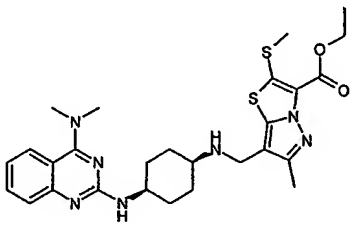
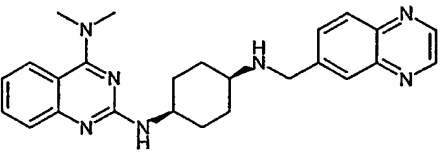
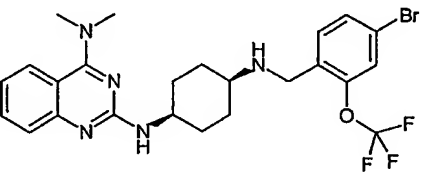
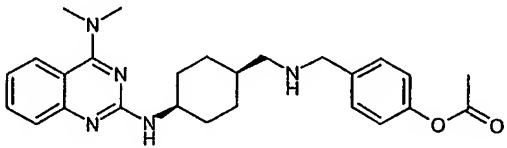
Example No.	Structure	APCI-MS
1937		588 (M + H)
1938		468 (M + H)
1939		443 (M + H)
1940		434 (M + H)
1941		500 (M + H)

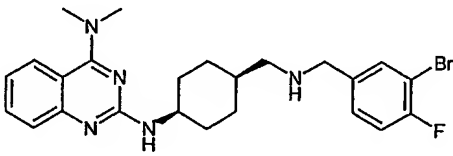
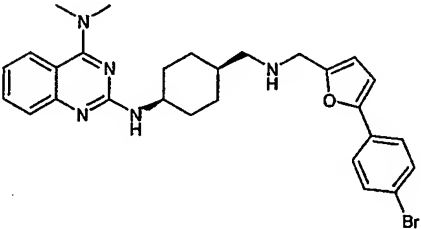
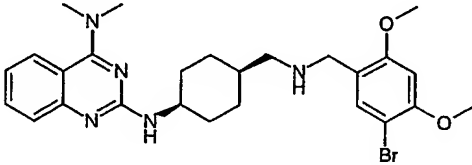
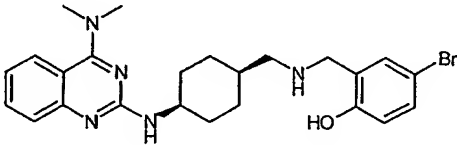
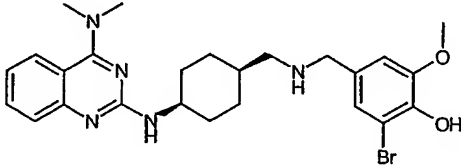
Example No.	Structure	APCI-MS
1942		530 (M + H)
1943		506 (M + H)
1944		414 (M + H)
1945		442 (M + H)
1946		448 (M + H)

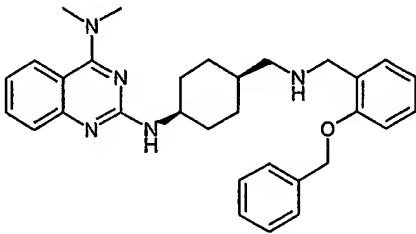
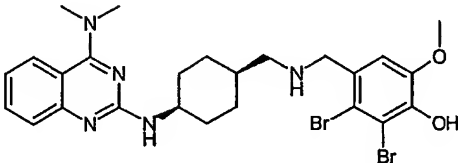
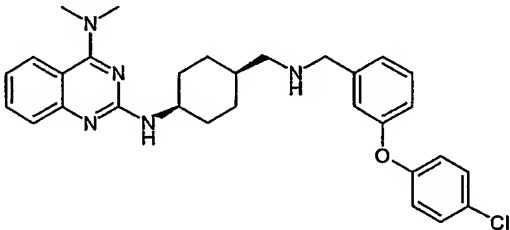
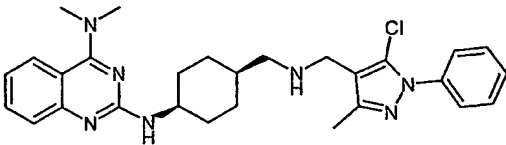
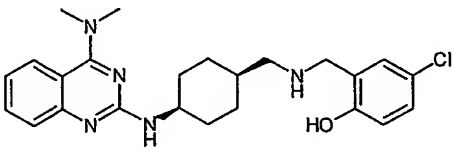
Example No.	Structure	APCI-MS
1947		474 (M + H)
1948		461 (M + H)
1949		509 (M + H)
1950		437 (M + H)
1951		427 (M + H)

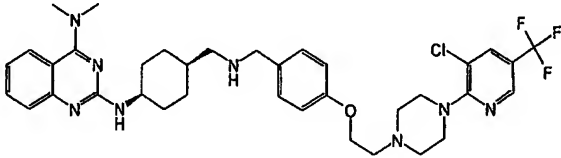
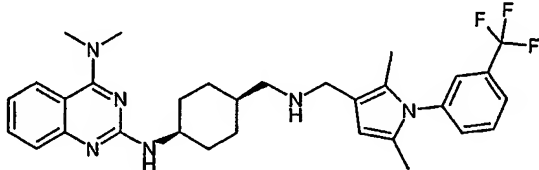
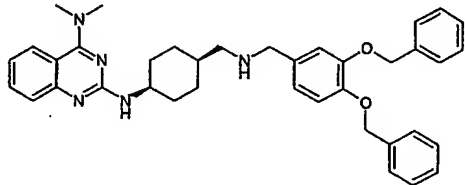
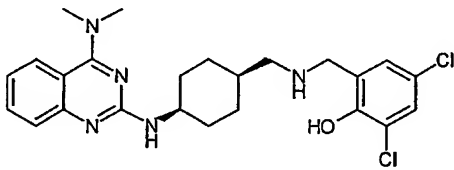
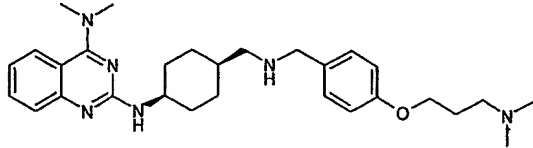
Example No.	Structure	APCI-MS
1952		444 (M + H)
1953		460 (M + H)
1954		447 (M + H)
1955		456 (M + H)
1956		479 (M + H)

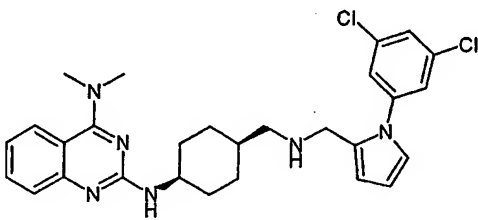
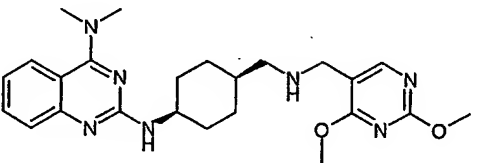
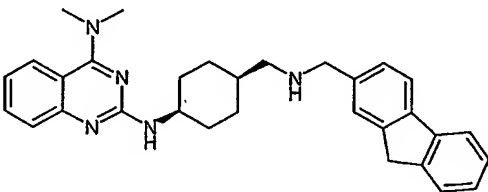
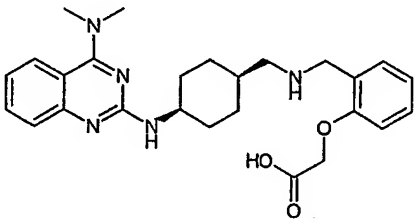
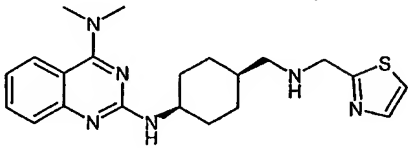
Example No.	Structure	APCI-MS
1957		469 (M + H)
1958		440 (M + H)
1959		476 (M + H)
1960		453 (M + H)
1961		552 (M + H)

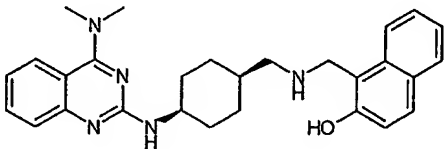
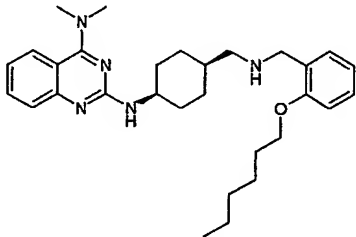
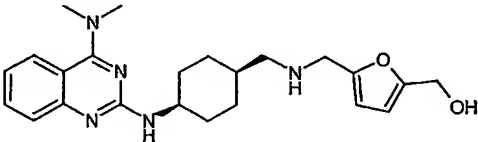
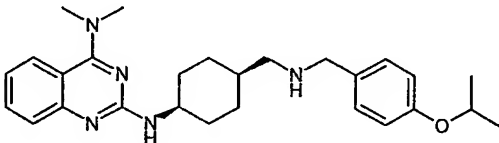
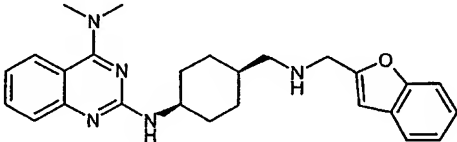
Example No.	Structure	APCI-MS
1962		500 (M + H)
1963		554 (M + H)
1964		428 (M + H)
1965		538 (M + H)
1966		448 (M + H)

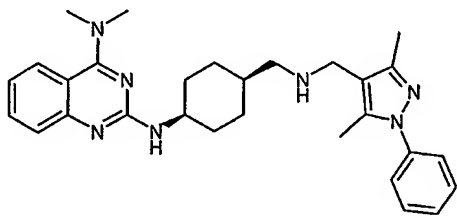
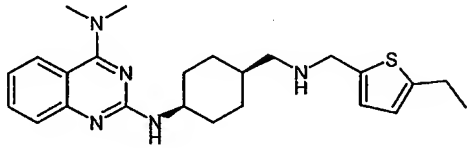
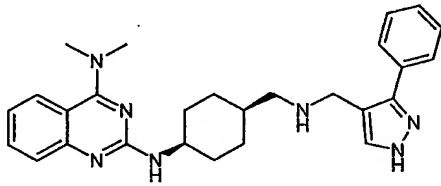
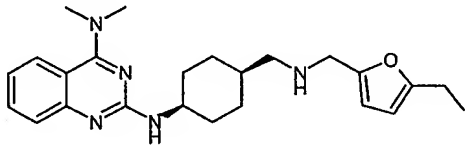
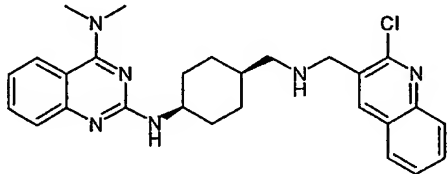
Example No.	Structure	APCI-MS
1967		486 (M + H)
1968		534 (M + H)
1969		528 (M + H)
1970		484 (M + H)
1971		514 (M + H)

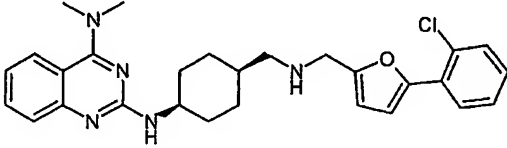
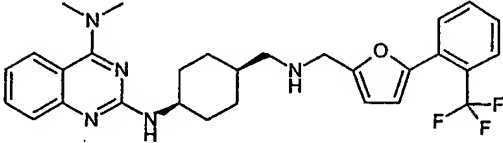
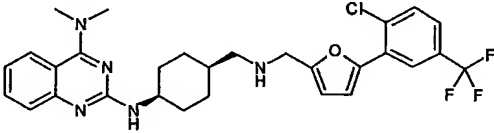
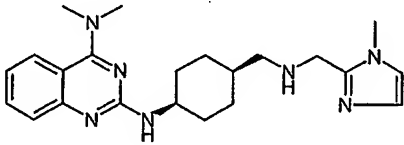
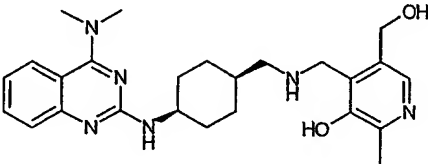
Example No.	Structure	APCI-MS
1972		496 (M + H)
1973		592 (M + H)
1974		516 (M + H)
1975		504 (M + H)
1976		440 (M + H)

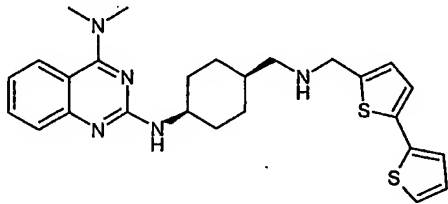
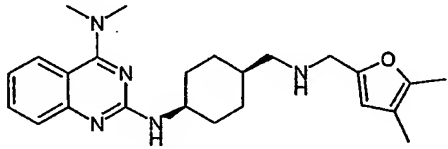
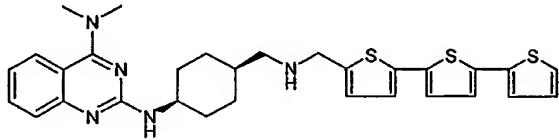
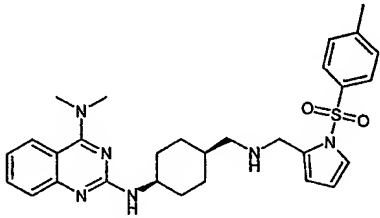
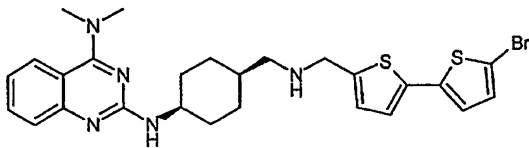
Example No.	Structure	APCI-MS
1977		697 (M + H)
1978		551 (M + H)
1979		602 (M + H)
1980		474 (M + H)
1981		491 (M + H)

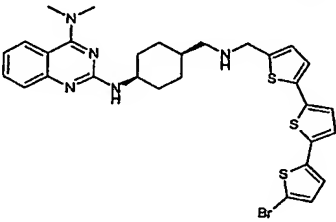
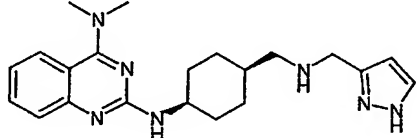
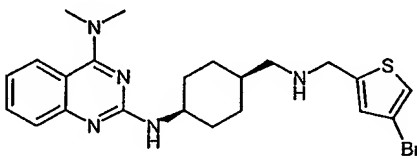
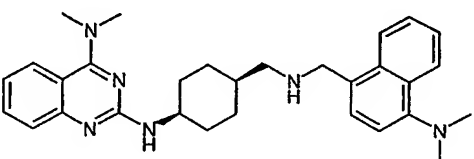
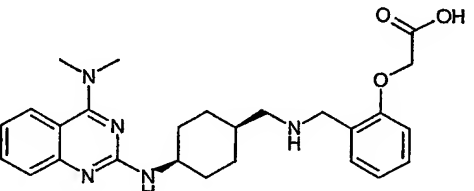
Example No.	Structure	APCI-MS
1982		523 (M + H)
1983		452 (M + H)
1984		478 (M + H)
1985		464 (M + H)
1986		397 (M + H)

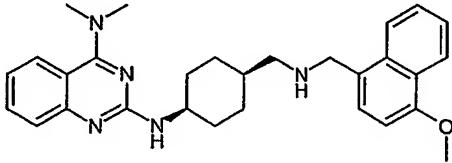
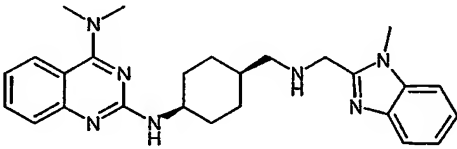
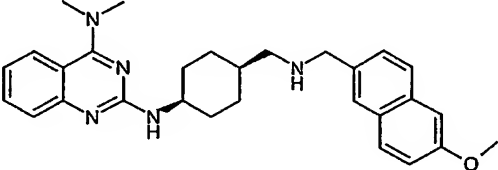
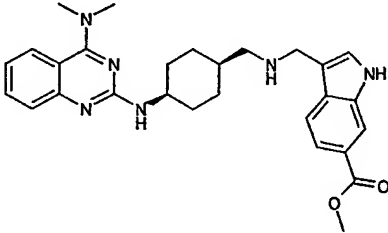
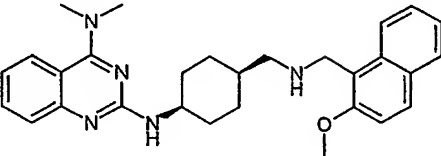
Example No.	Structure	APCI-MS
1987		454 (M - H)
1988		490 (M + H)
1989		410 (M + H)
1990		448 (M + H)
1991		430 (M + H)

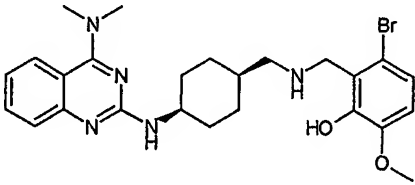
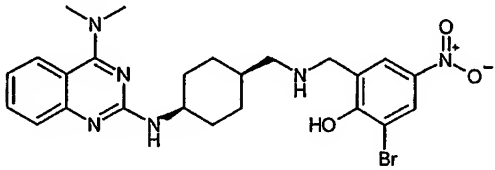
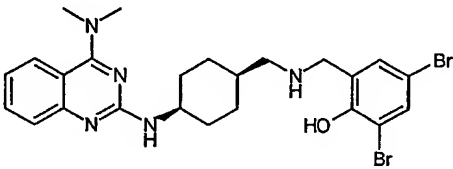
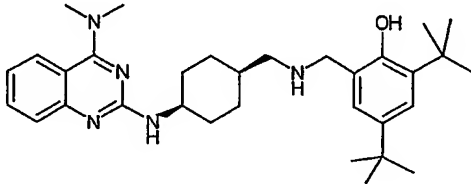
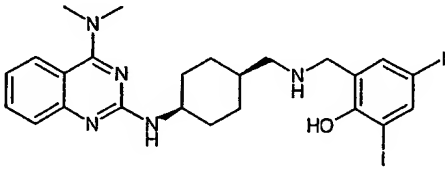
Example No.	Structure	APCI-MS
1992		484 (M + H)
1993		424 (M + H)
1994		456 (M + H)
1995		408 (M + H)
1996		475 (M + H)

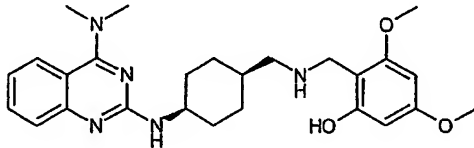
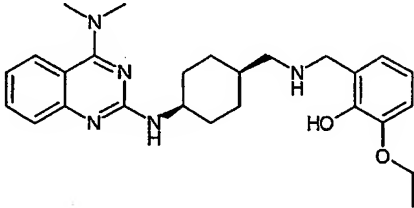
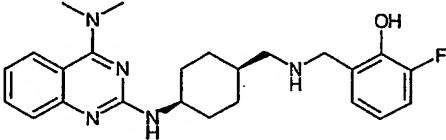
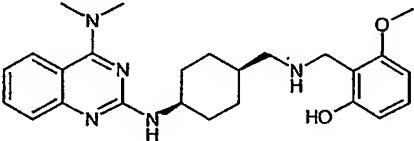
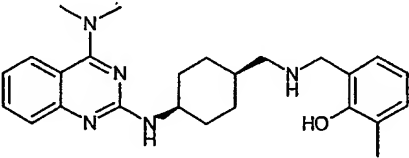
Example No.	Structure	APCI-MS
1997		490 (M + H)
1998		524 (M + H)
1999		558 (M + H)
2000		394 (M + H)
2001		451 (M + H)

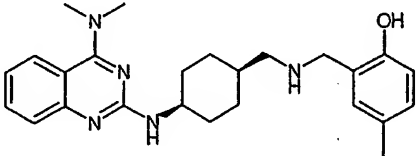
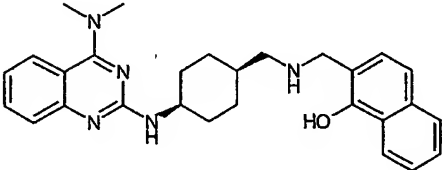
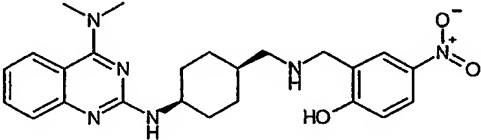
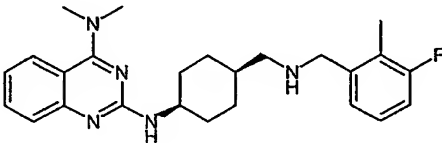
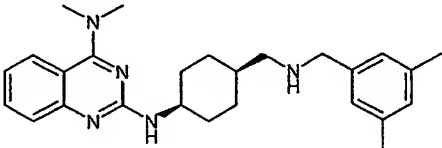
Example No.	Structure	APCI-MS
2002		478 (M + H)
2003		408 (M + H)
2004		560 (M + H)
2005		533 (M + H)
2006		556 (M + H)

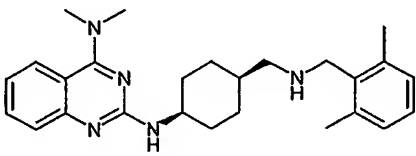
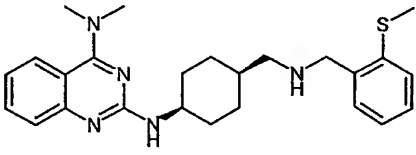
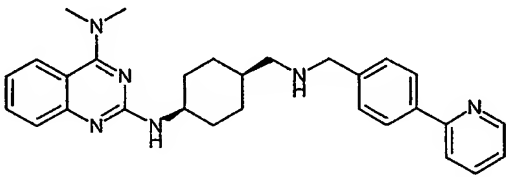
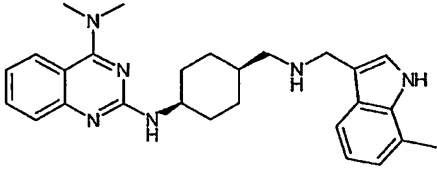
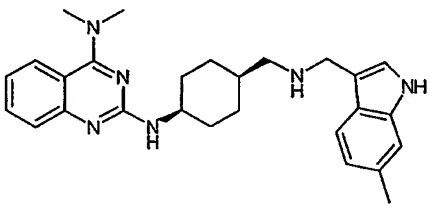
Example No.	Structure	APCI-MS
2007		638 (M + H)
2008		380 (M + H)
2009		474 (M + H)
2010		483 (M + H)
2011		464 (M + H)

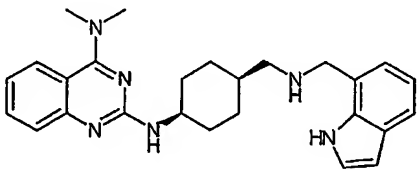
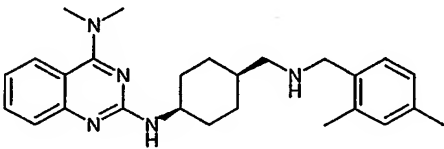
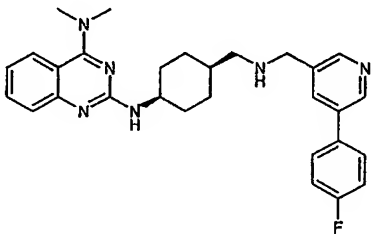
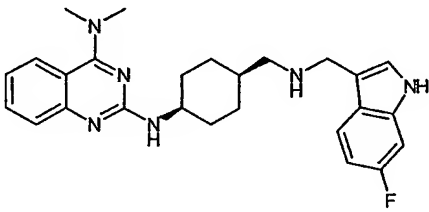
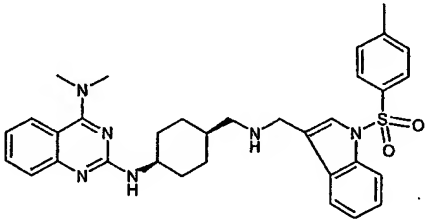
Example No.	Structure	APCI-MS
2012		470 (M + H)
2013		444 (M + H)
2014		470 (M + H)
2015		487 (M + H)
2016		470 (M + H)

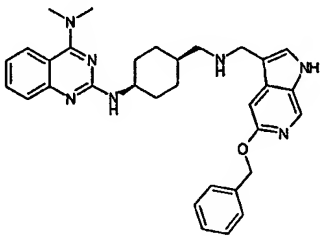
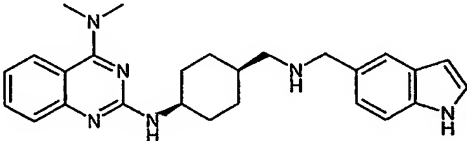
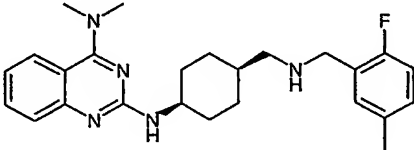
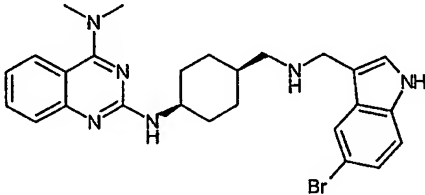
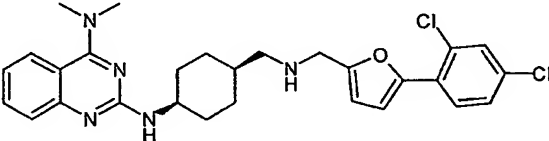
Example No.	Structure	APCI-MS
2017		514 (M + H)
2018		527 (M - H)
2019		562 (M + H)
2020		518 (M + H)
2021		658 (M + H)

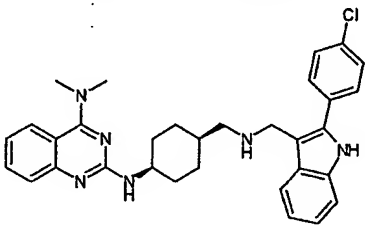
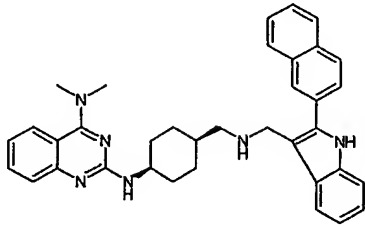
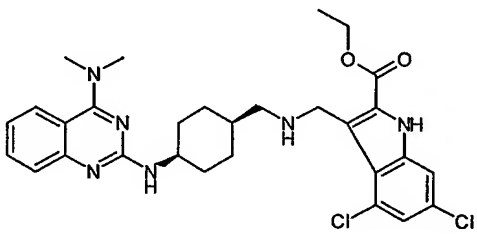
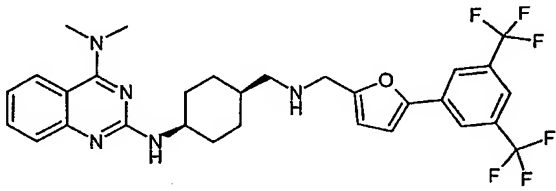
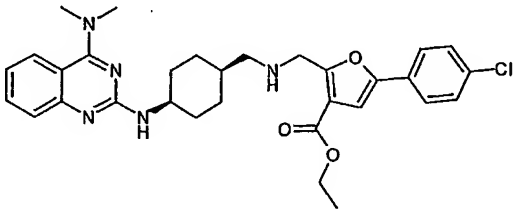
Example No.	Structure	APCI-MS
2022		466 (M + H)
2023		450 (M + H)
2024		424 (M + H)
2025		436 (M + H)
2026		420 (M + H)

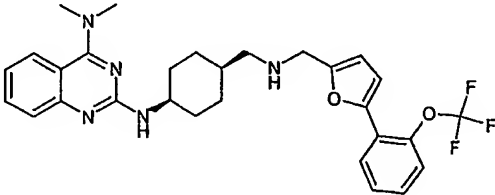
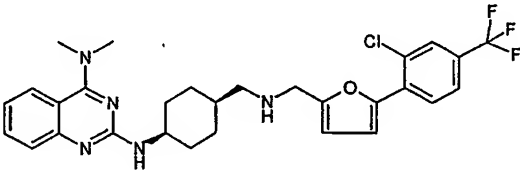
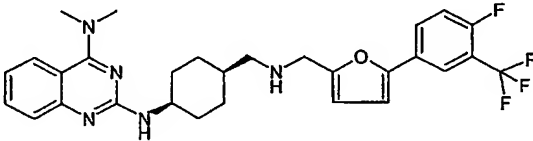
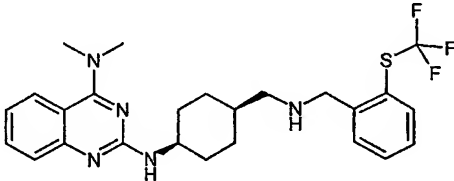
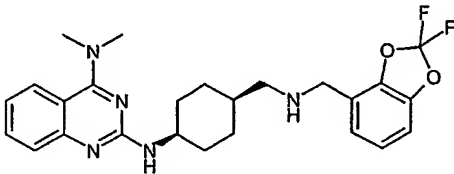
Example No.	Structure	APCI-MS
2027		420 (M + H)
2028		456 (M + H)
2029		451 (M + H)
2030		422 (M + H)
2031		418 (M + H)

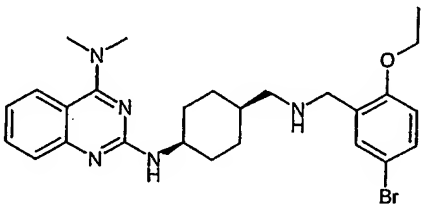
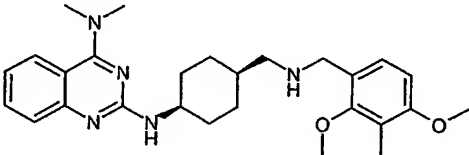
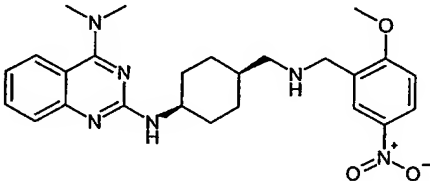
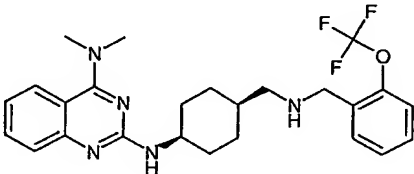
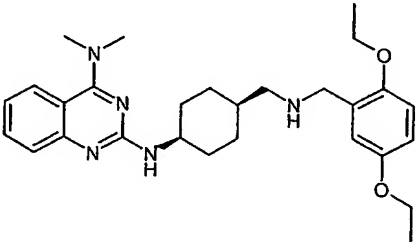
Example No.	Structure	APCI-MS
2032		418 (M + H)
2033		436 (M + H)
2034		467 (M + H)
2035		443 (M + H)
2036		443 (M + H)

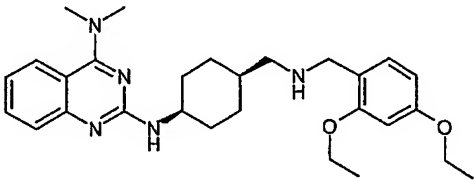
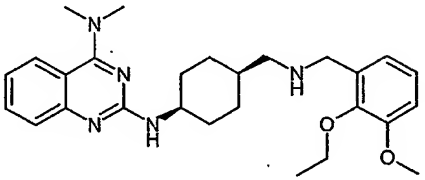
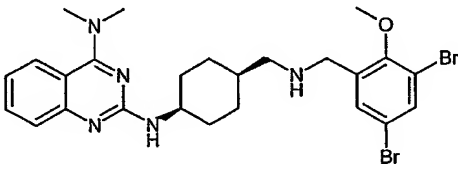
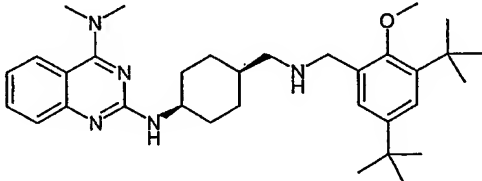
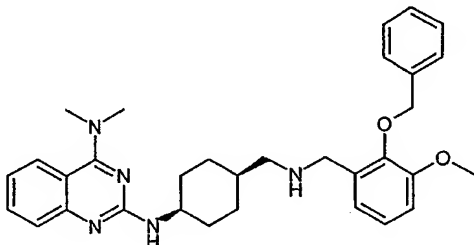
Example No.	Structure	APCI-MS
2037		429 (M + H)
2038		418 (M + H)
2039		485 (M + H)
2040		447 (M + H)
2041		583 (M + H)

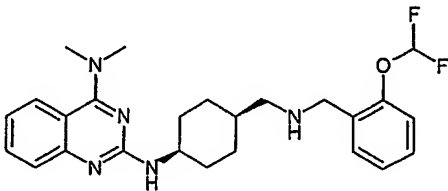
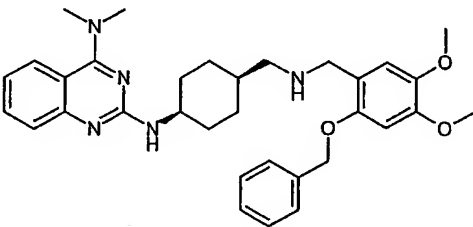
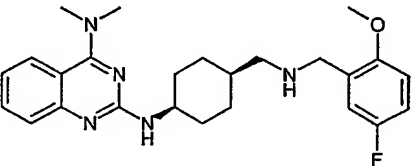
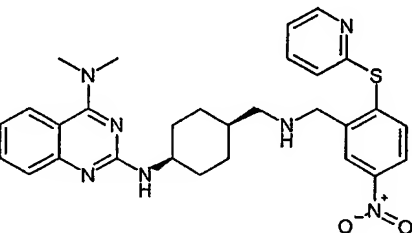
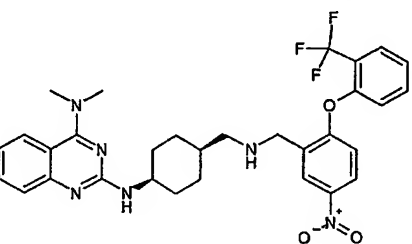
Example No.	Structure	APCI-MS
2042		536 (M + H)
2043		429 (M + H)
2044		422 (M + H)
2045		507 (M + H)
2046		524 (M + H)

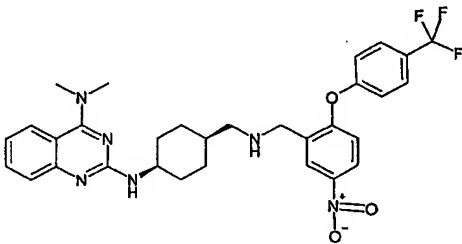
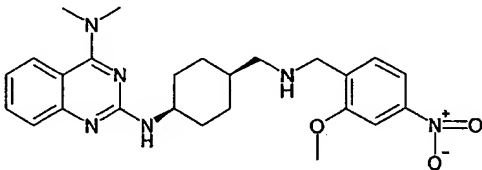
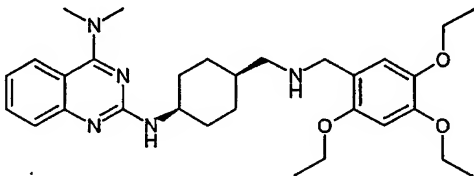
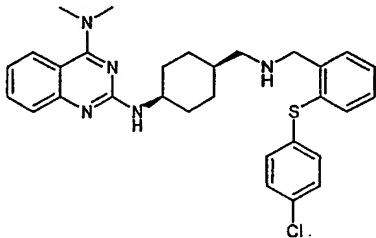
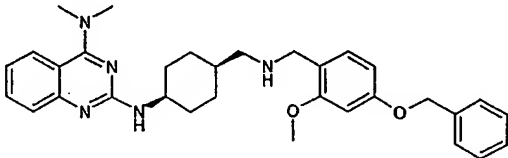
Example No.	Structure	APCI-MS
2047		539 (M + H)
2048		555 (M + H)
2049		569 (M + H)
2050		592 (M + H)
2051		562 (M + H)

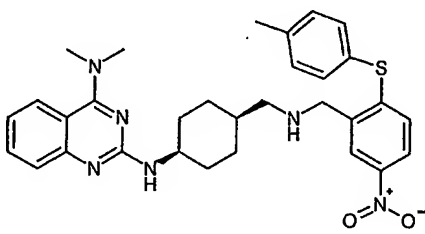
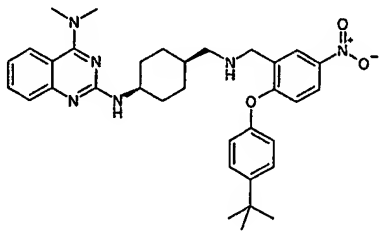
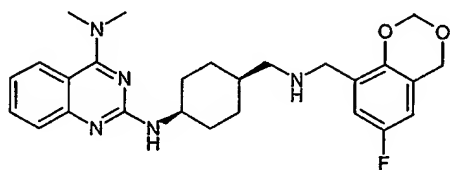
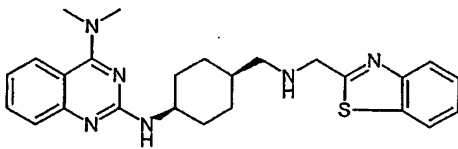
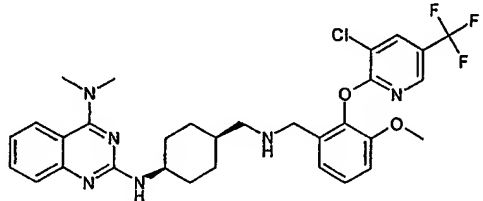
Example No.	Structure	APCI-MS
2052		540 (M + H)
2053		558 (M + H)
2054		542 (M + H)
2055		490 (M + H)
2056		470 (M + H)

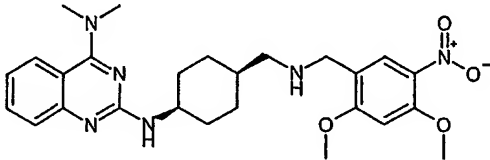
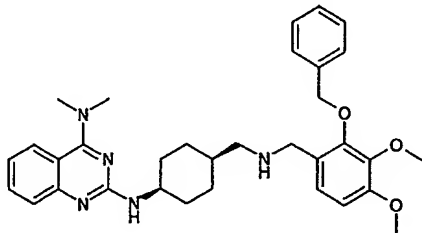
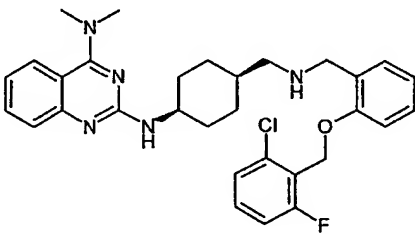
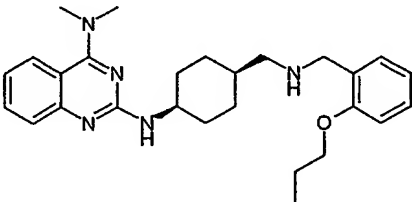
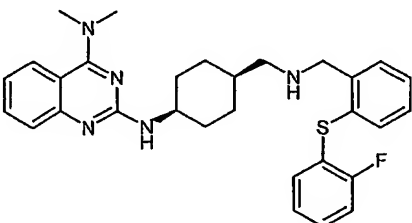
Example No.	Structure	APCI-MS
2057		512 (M + H)
2058		464 (M + H)
2059		465 (M + H)
2060		474 (M + H)
2061		478 (M + H)

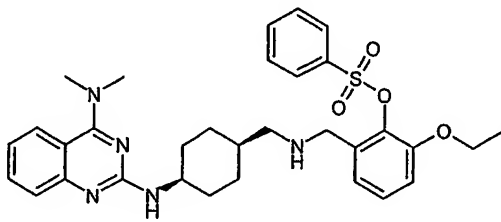
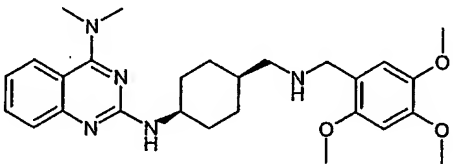
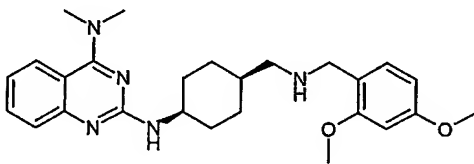
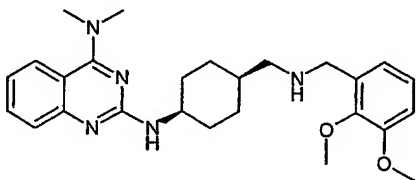
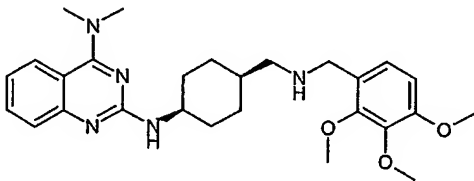
Example No.	Structure	APCI-MS
2062		478 (M + H)
2063		464 (M + H)
2064		576 (M + H)
2065		532 (M + H)
2066		526 (M + H)

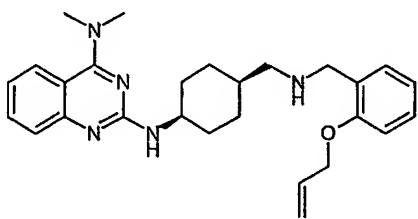
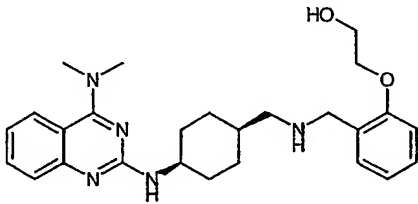
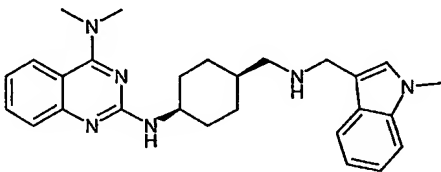
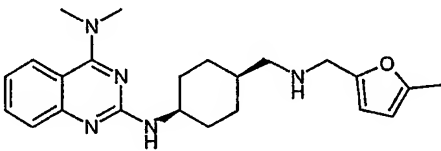
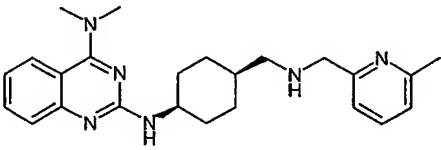
Example No.	Structure	APCI-MS
2067		456 (M + H)
2068		556 (M + H)
2069		438 (M + H)
2070		544 (M + H)
2071		595 (M + H)

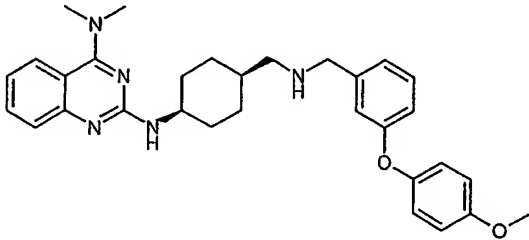
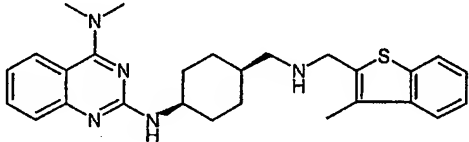
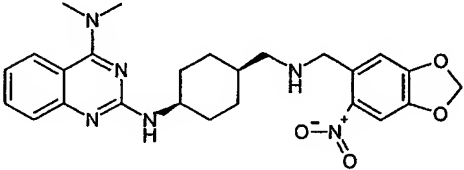
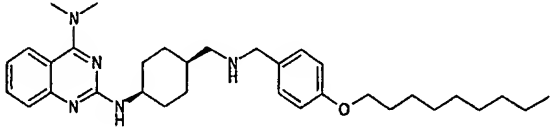
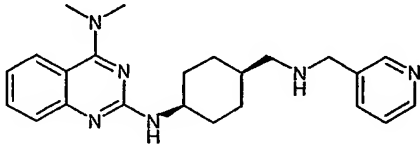
Example No.	Structure	APCI-MS
2072		595 (M + H)
2073		465 (M + H)
2074		522 (M + H)
2075		532 (M + H)
2076		526 (M + H)

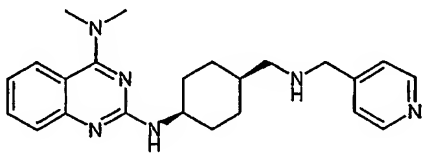
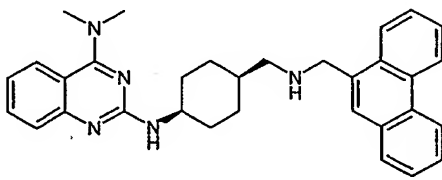
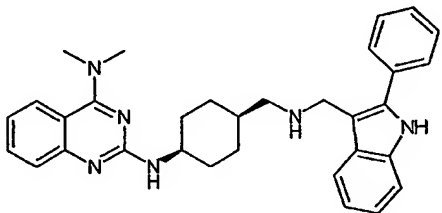
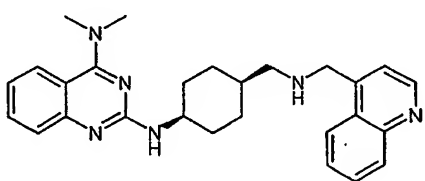
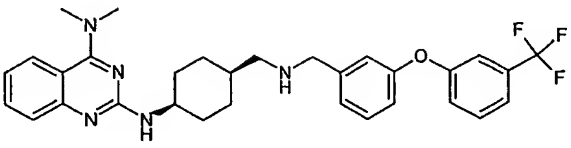
Example No.	Structure	APCI-MS
2077		557 (M + H)
2078		583 (M + H)
2079		466 (M + H)
2080		447 (M + H)
2081		615 (M + H)

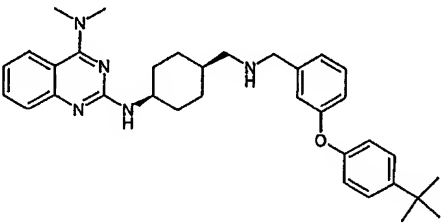
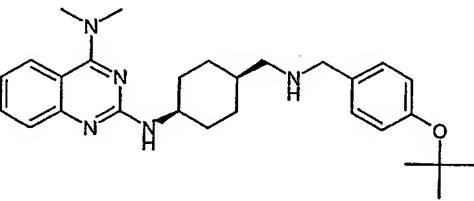
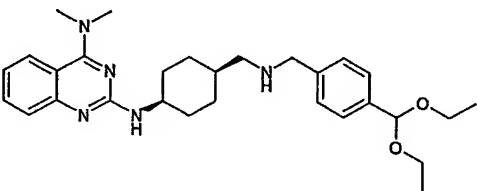
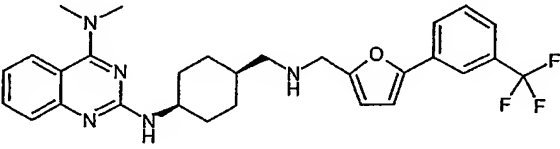
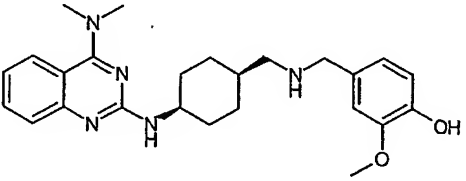
Example No.	Structure	APCI-MS
2082		495 (M + H)
2083		556 (M + H)
2084		548 (M + H)
2085		448 (M + H)
2086		516 (M + H)

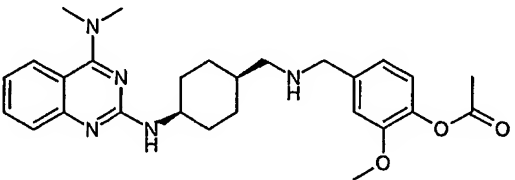
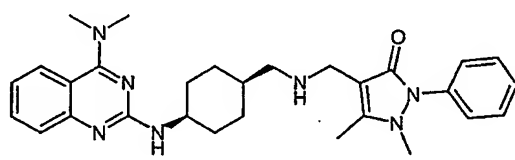
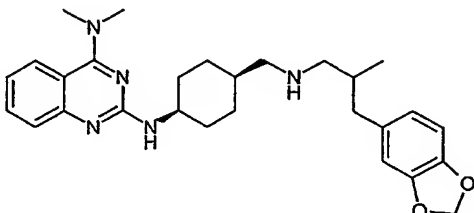
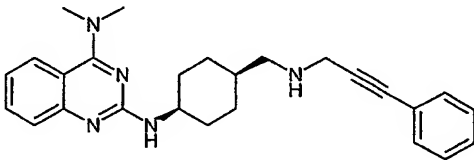
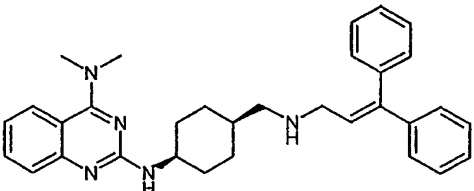
Example No.	Structure	APCI-MS
2087		590 (M + H)
2088		480 (M + H)
2089		450 (M + H)
2090		450 (M + H)
2091		480 (M + H)

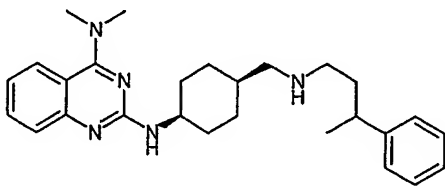
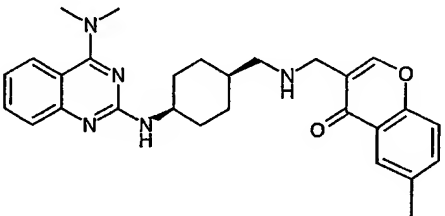
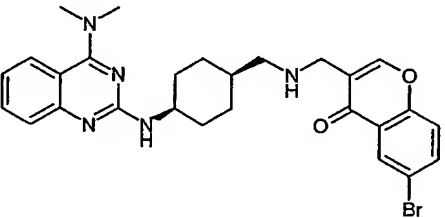
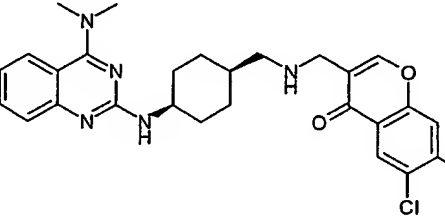
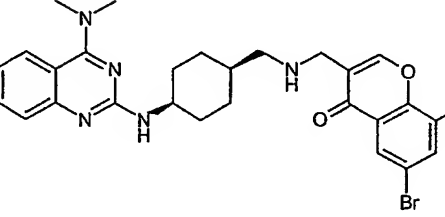
Example No.	Structure	APCI-MS
2092		446 (M + H)
2093		450 (M + H)
2094		443 (M + H)
2095		394 (M + H)
2096		405 (M + H)

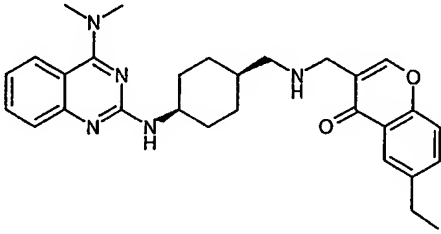
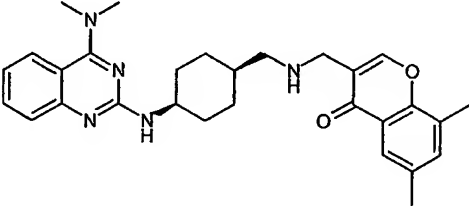
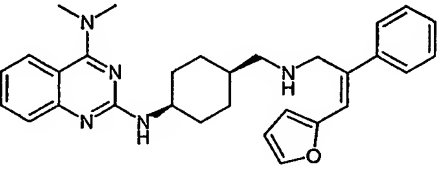
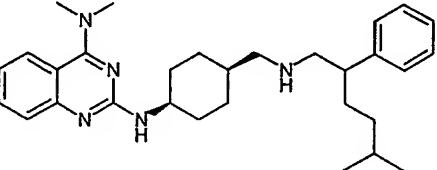
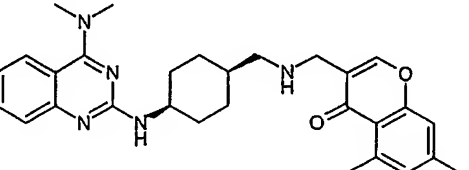
Example No:	Structure	APCI-MS
2097		512 (M + H)
2098		460 (M + H)
2099		479 (M + H)
2100		532 (M + H)
2101		391 (M + H)

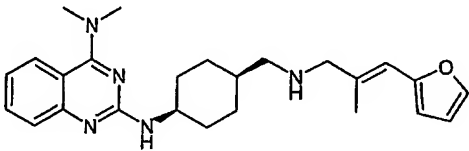
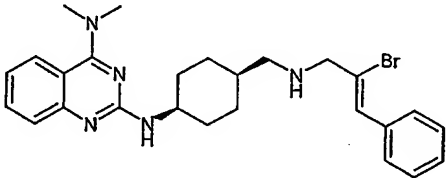
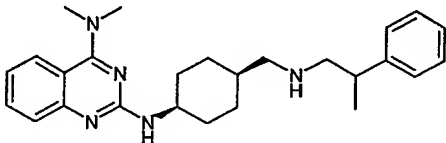
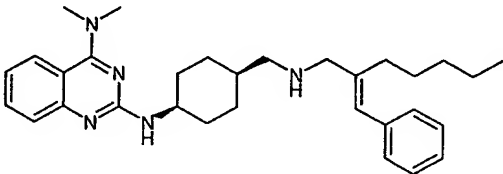
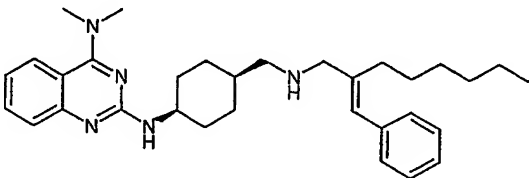
Example No.	Structure	APCI-MS
2102		391 (M + H)
2103		490 (M + H)
2104		505 (M + H)
2105		441 (M + H)
2106		550 (M + H)

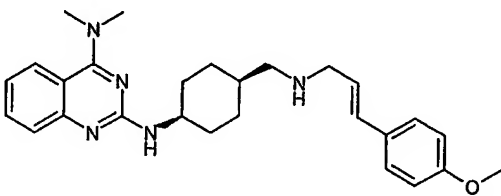
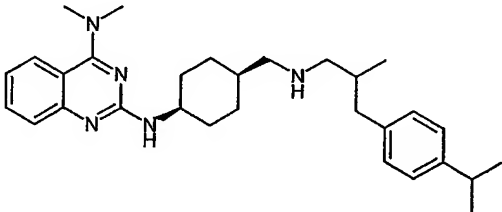
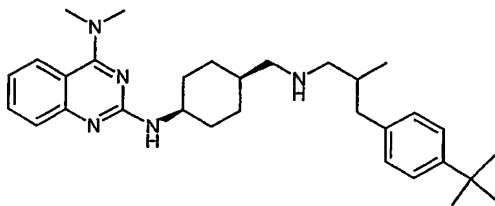
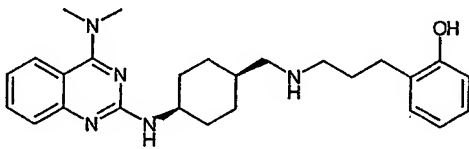
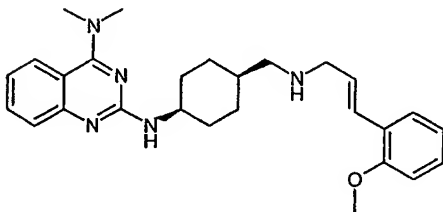
Example No.	Structure	APCI-MS
2107		538 (M + H)
2108		462 (M + H)
2109		492 (M + H)
2110		524 (M + H)
2111		436 (M + H)

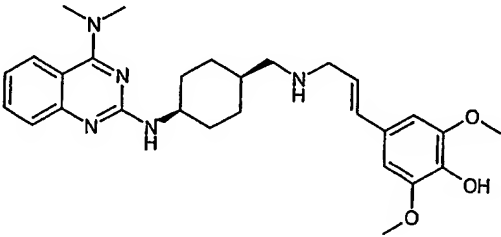
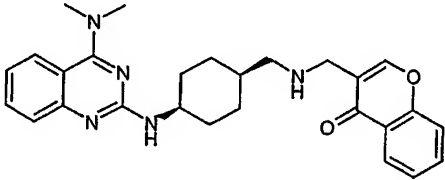
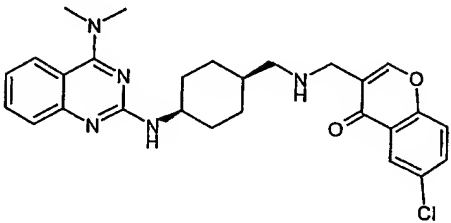
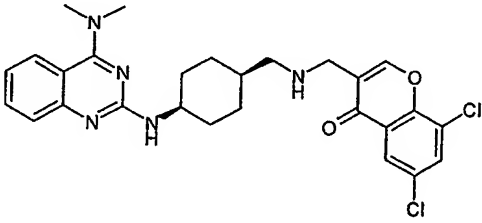
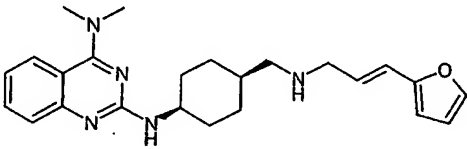
Example No.	Structure	APCI-MS
2112		478 (M + H)
2113		500 (M + H)
2114		476 (M + H)
2115		414 (M + H)
2116		492 (M + H)

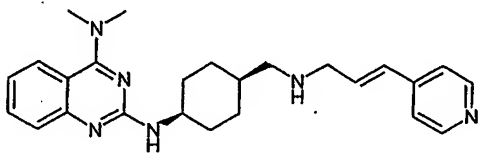
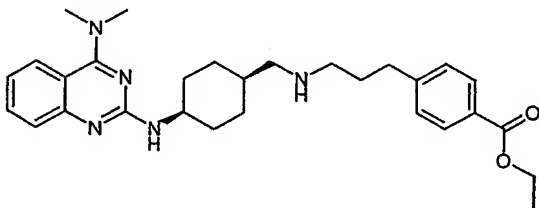
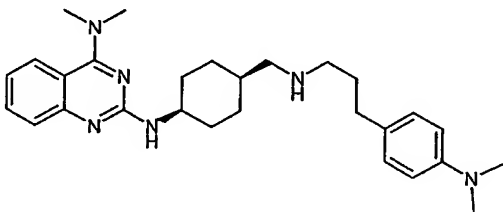
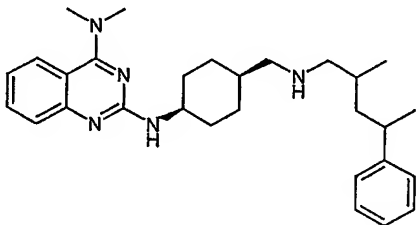
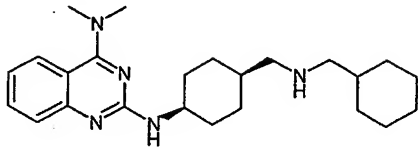
Example No.	Structure	APCI-MS
2117		432 (M + H)
2118		472 (M + H)
2119		536 (M + H)
2120		506 (M + H)
2121		614 (M + H)

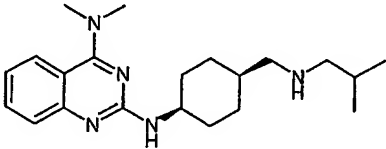
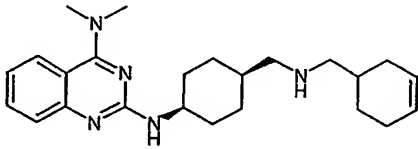
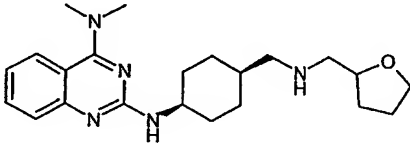
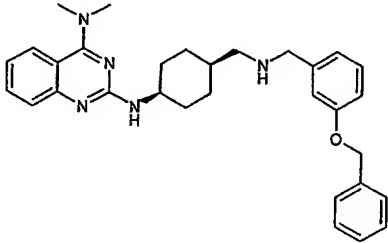
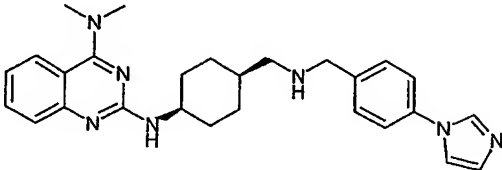
Example No.	Structure	APCI-MS
2122		486 (M + H)
2123		486 (M + H)
2124		482 (M + H)
2125		474 (M + H)
2126		486 (M + H)

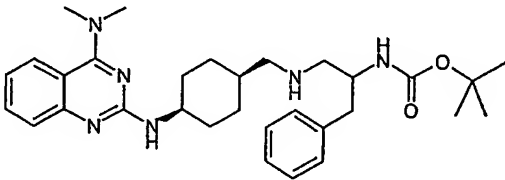
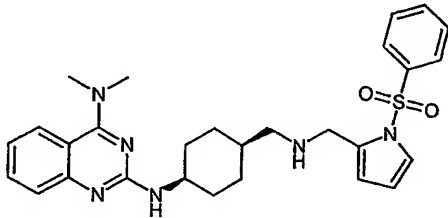
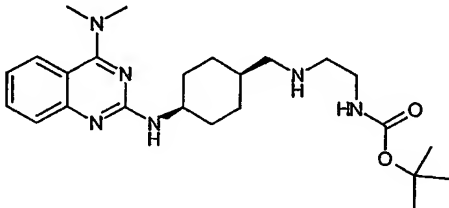
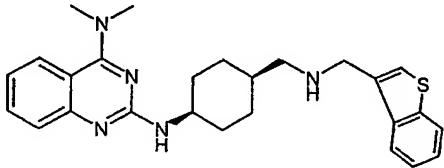
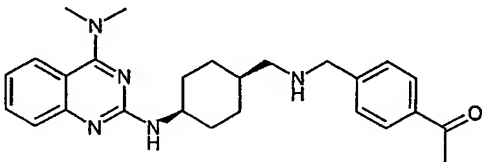
Example No.	Structure	APCI-MS
2127		420 (M + H)
2128		494 (M + H)
2129		418 (M + H)
2130		486 (M + H)
2131		500 (M + H)

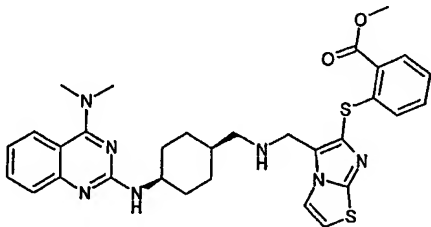
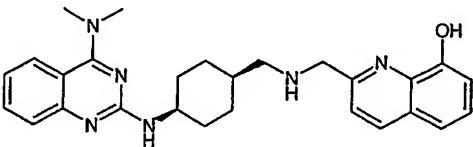
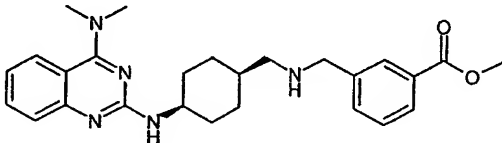
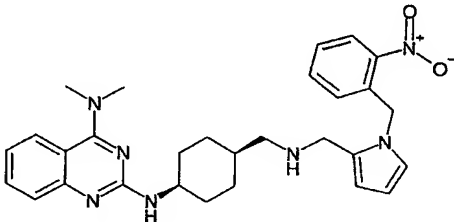
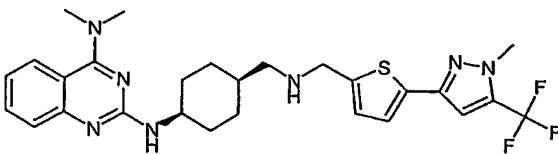
Example No.	Structure	APCI-MS
2132		446 (M + H)
2133		474 (M + H)
2134		488 (M + H)
2135		434 (M + H)
2136		446 (M + H)

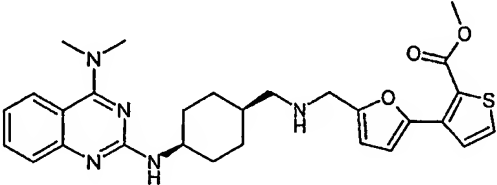
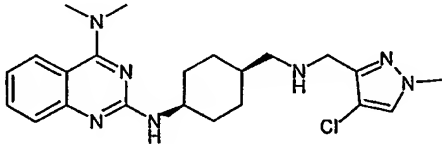
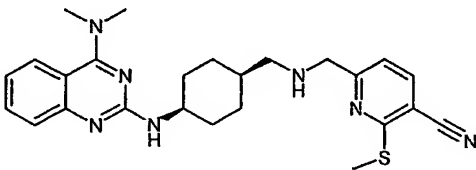
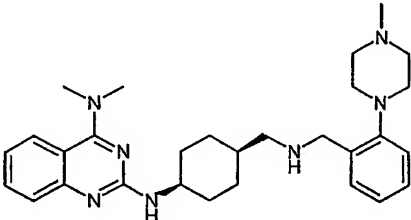
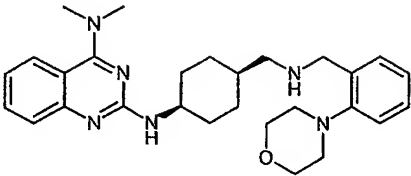
Example No.	Structure	APCI-MS
2137		492 (M + H)
2138		458 (M + H)
2139		492 (M + H)
2140		526 (M + H)
2141		406 (M + H)

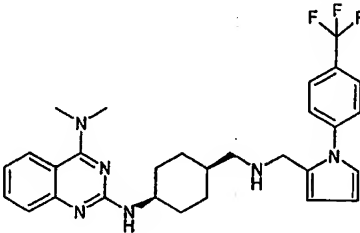
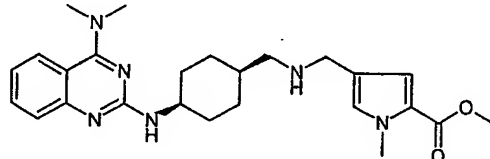
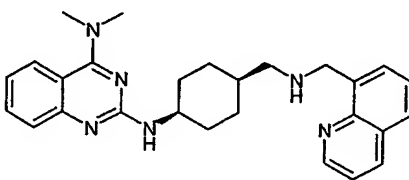
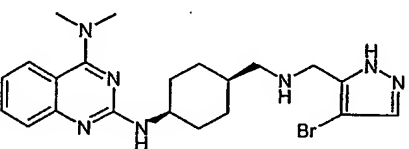
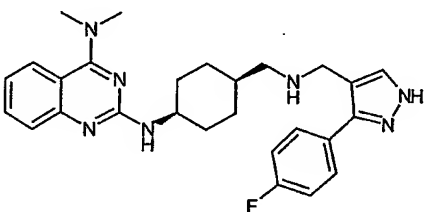
Example No.	Structure	APCI-MS
2142		417 (M + H)
2143		490 (M + H)
2144		461 (M + H)
2145		460 (M + H)
2146		396 (M + H)

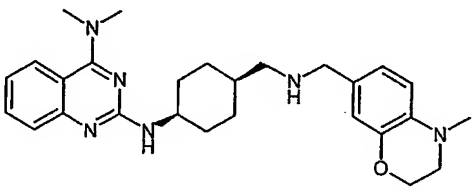
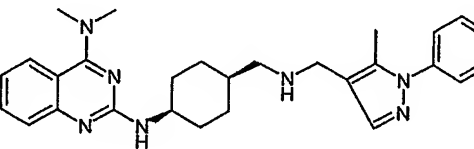
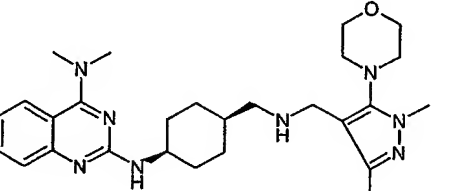
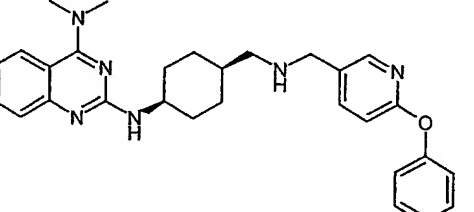
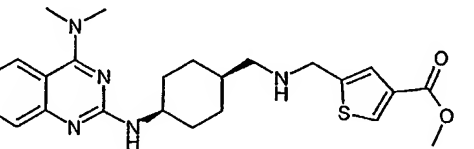
Example No.	Structure	APCI-MS
2147		356 (M + H)
2148		394 (M + H)
2149		384 (M + H)
2150		496 (M + H)
2151		456 (M + H)

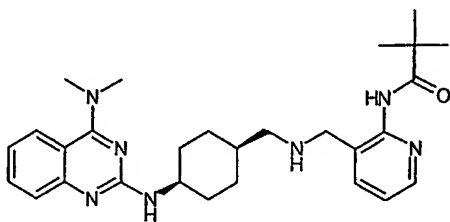
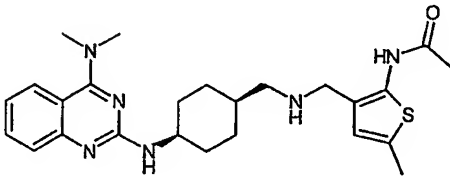
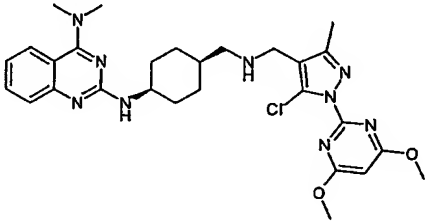
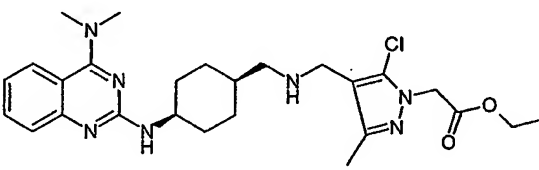
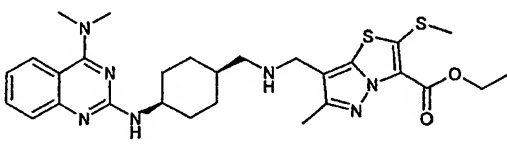
Example No.	Structure	APCI-MS
2152		533 (M + H)
2153		519 (M + H)
2154		443 (M + H)
2155		446 (M + H)
2156		432 (M + H)

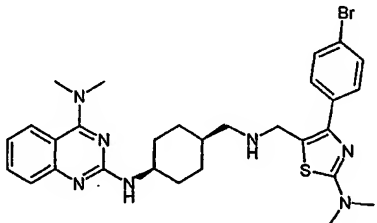
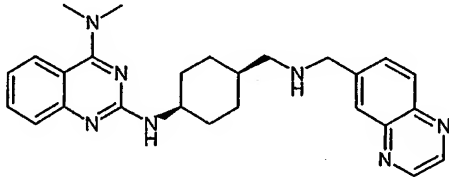
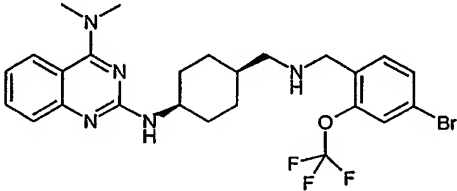
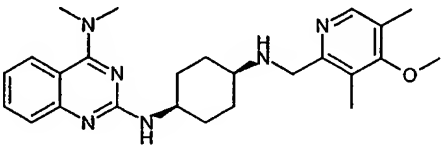
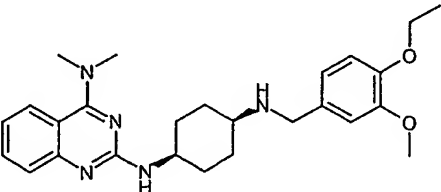
Example No.	Structure	APCI-MS
2157		602 (M + H)
2158		457 (M + H)
2159		448 (M + H)
2160		514 (M + H)
2161		544 (M + H)

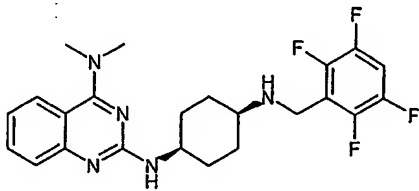
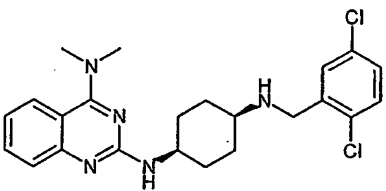
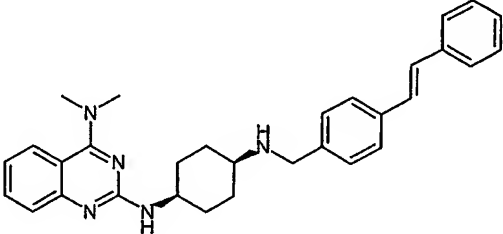
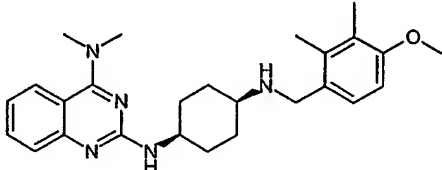
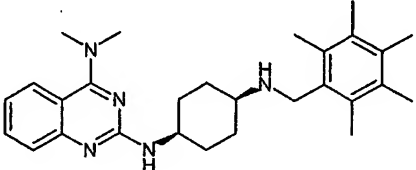
Example No.	Structure	APCI-MS
2162		520 (M + H)
2163		428 (M + H)
2164		462 (M + H)
2165		488 (M + H)
2166		475 (M + H)

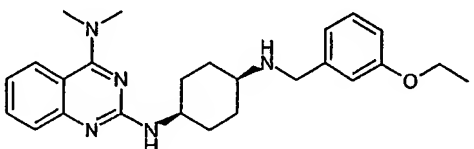
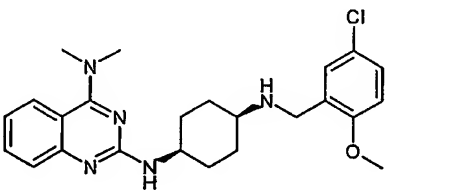
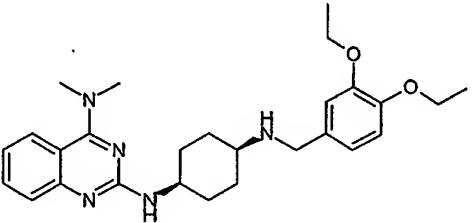
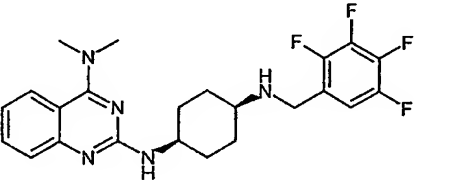
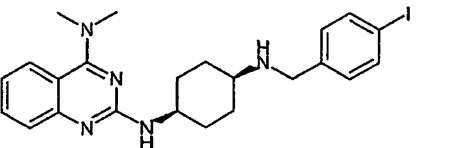
Example No.	Structure	APCI-MS
2167		523 (M + H)
2168		451 (M + H)
2169		441 (M + H)
2170		458 (M + H)
2171		474 (M + H)

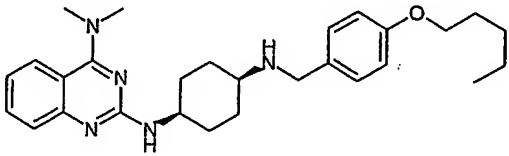
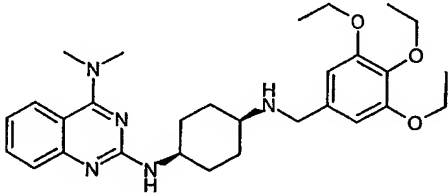
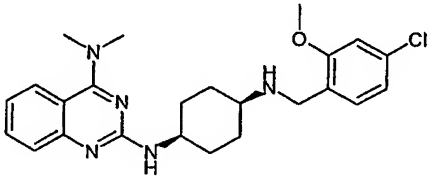
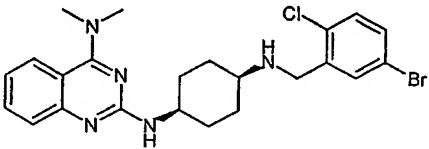
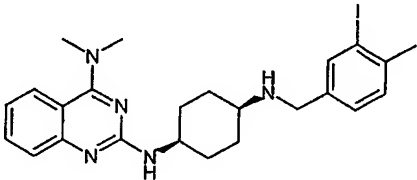
Example No.	Structure	APCI-MS
2172		461 (M + H)
2173		470 (M + H)
2174		493 (M + H)
2175		483 (M + H)
2176		454 (M + H)

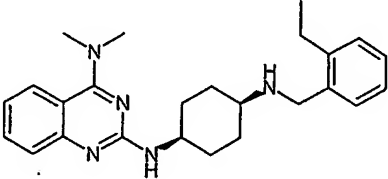
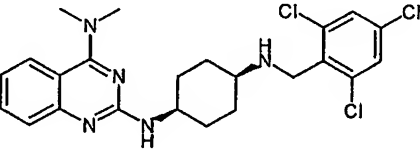
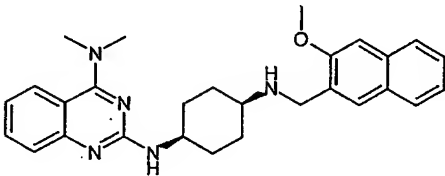
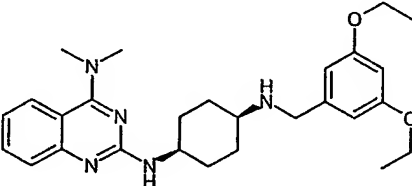
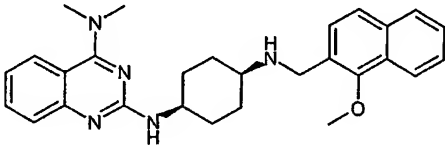
Example No.	Structure	APCI-MS
2177		490 (M + H)
2178		467 (M + H)
2179		566 (M + H)
2180		514 (M + H)
2181		568 (M + H)

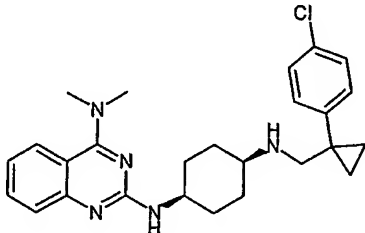
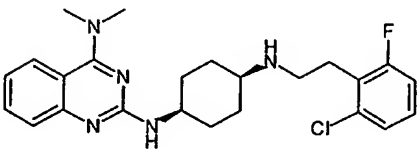
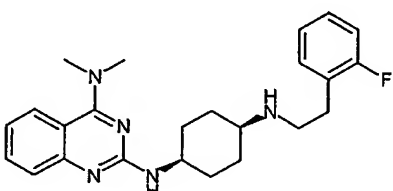
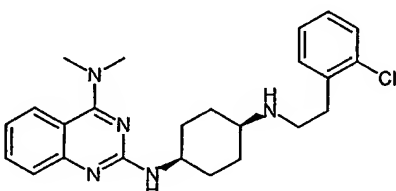
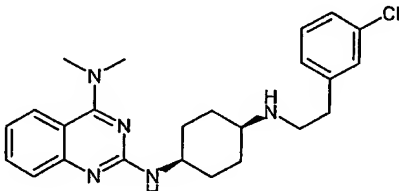
Example No.	Structure	APCI-MS
2182		594 (M + H)
2183		442 (M + H)
2184		552 (M + H)
2185		435 (M + H)
2186		450 (M + H)

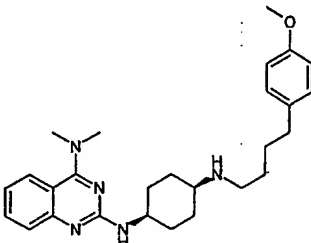
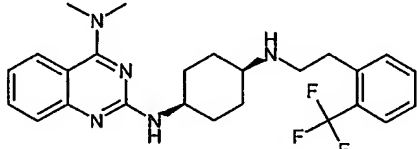
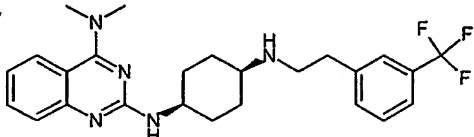
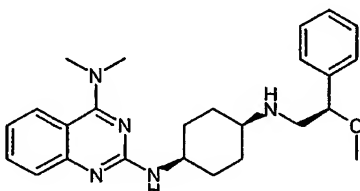
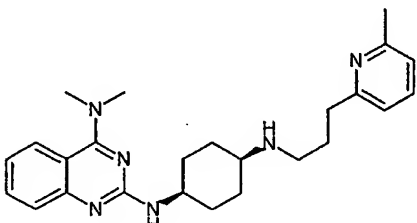
Example No.	Structure	APCI-MS
2187		448 (M + H)
2188		444 (M + H)
2189		478 (M + H)
2190		434 (M + H)
2191		446 (M + H)

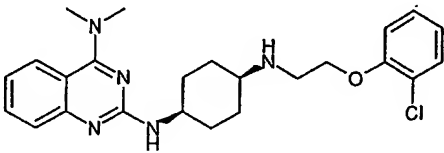
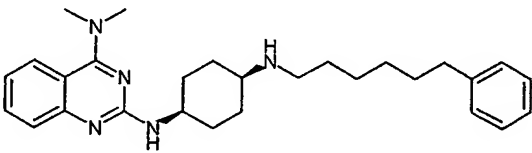
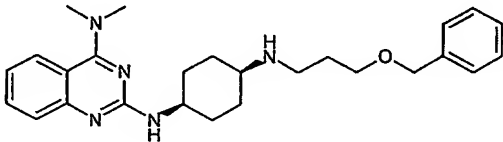
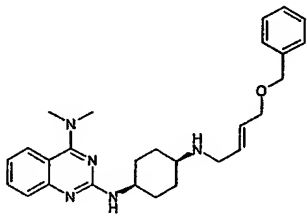
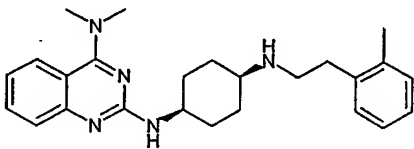
Example No.	Structure	APCI-MS
2192		420 (M + H)
2193		440 (M + H)
2194		464 (M + H)
2195		448 (M + H)
2196		502 (M + H)

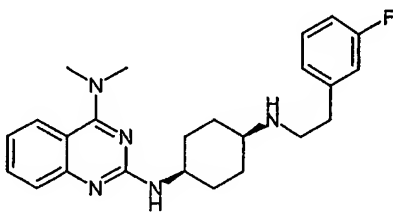
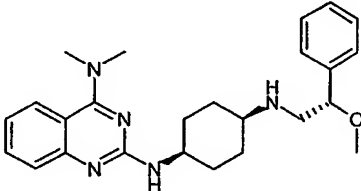
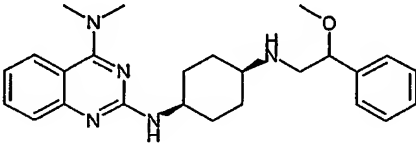
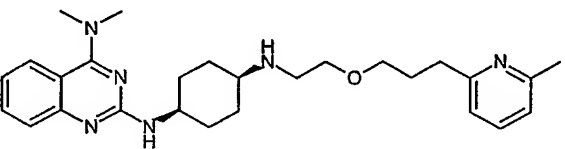
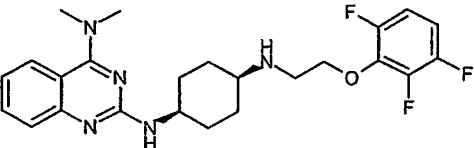
Example No.	Structure	APCI-MS
2197		462 (M + H)
2198		508 (M + H)
2199		440 (M + H)
2200		488 (M + H)
2201		516 (M + H)

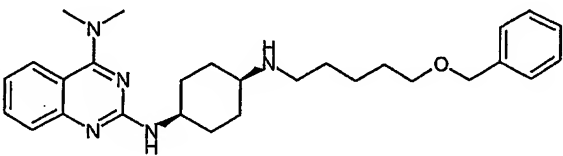
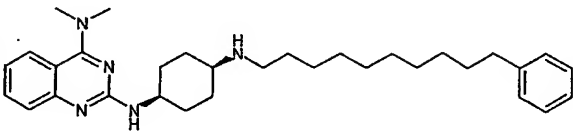
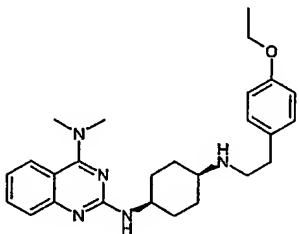
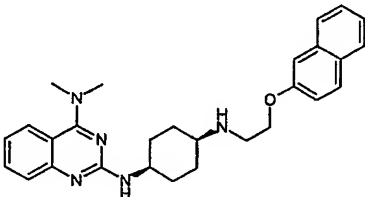
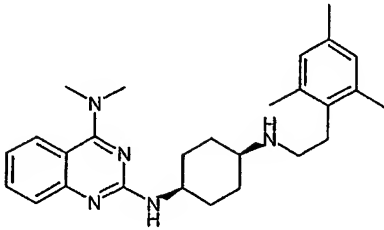
Example No.	Structure	APCI-MS
2202		404 (M + H)
2203		478 (M + H)
2204		456 (M + H)
2205		464 (M + H)
2206		456 (M + H)

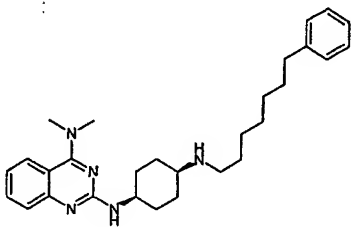
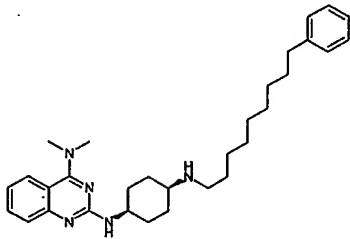
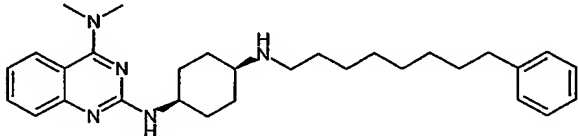
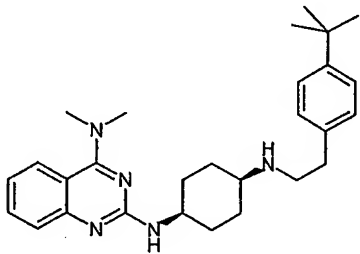
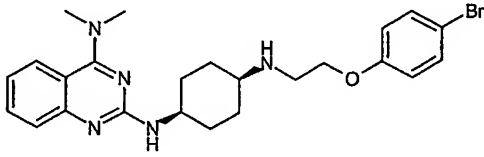
Example No.	Structure	APCI-MS
2207		450 (M + H)
2208		442 (M + H)
2209		408 (M + H)
2210		424 (M + H)
2211		424 (M + H)

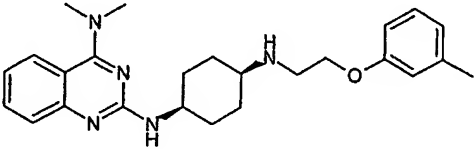
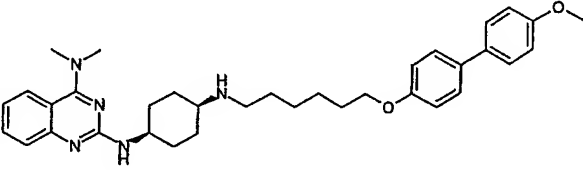
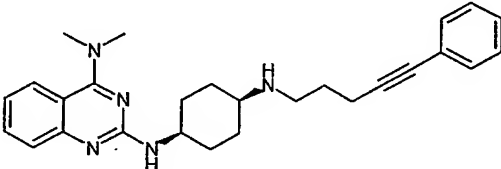
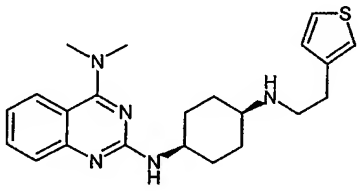
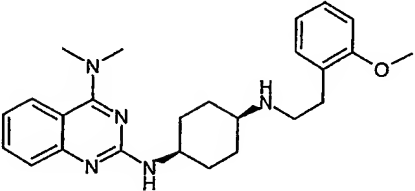
Example No.	Structure	APCI-MS
2212		448 (M + H)
2213		458 (M + H)
2214		458 (M + H)
2215		420 (M + H)
2216		419 (M + H)

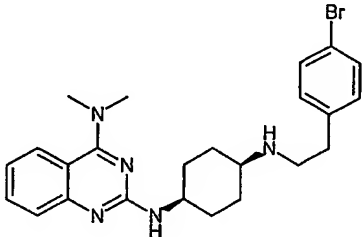
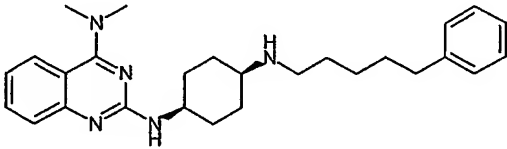
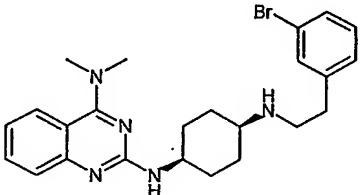
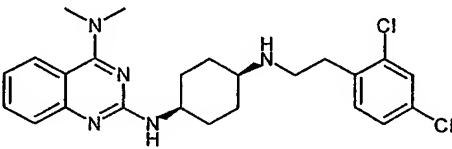
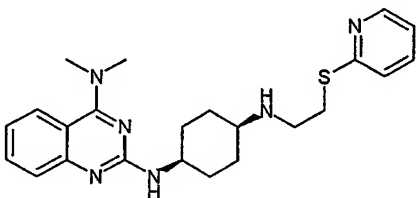
Example No.	Structure	APCI-MS
2217		440 (M + H)
2218		446 (M + H)
2219		434 (M + H)
2220		446 (M + H)
2221		404 (M + H)

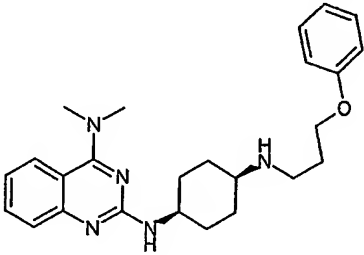
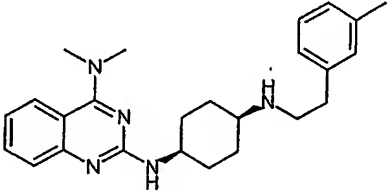
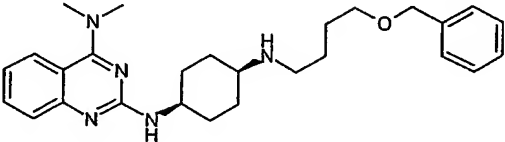
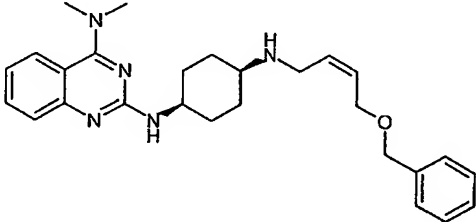
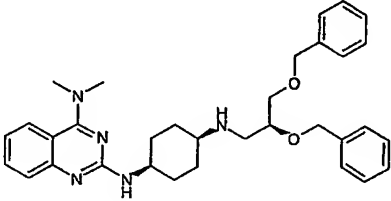
Example No.	Structure	APCI-MS
2222		408 (M + H)
2223		420 (M + H)
2224		420 (M + H)
2225		463 (M + H)
2226		460 (M + H)

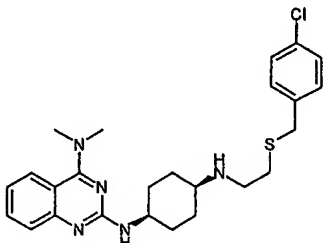
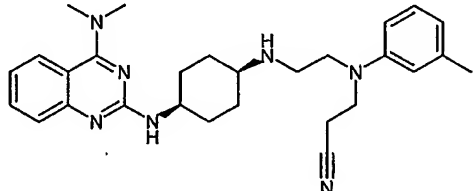
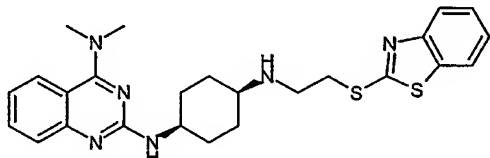
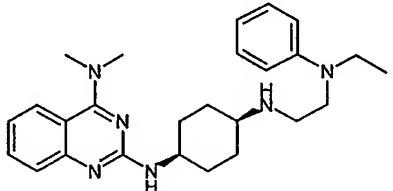
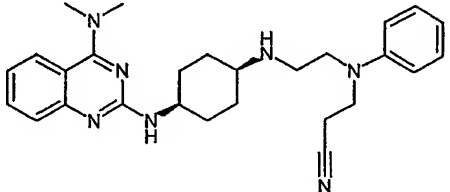
Example No.	Structure	APCI-MS
2227		462 (M + H)
2228		502 (M + H)
2229		434 (M + H)
2230		456 (M + H)
2231		432 (M + H)

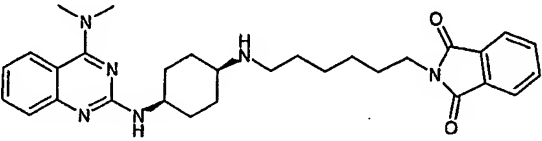
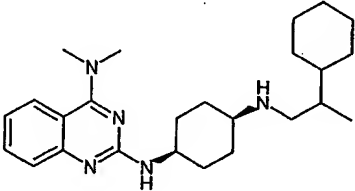
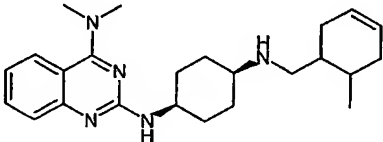
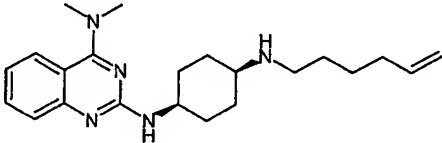
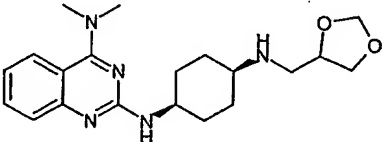
Example No.	Structure	APCI-MS
2232		460 (M + H)
2233		488 (M + H)
2234		474 (M + H)
2235		446 (M + H)
2236		484 (M + H)

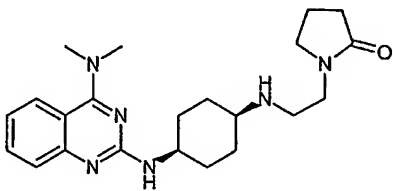
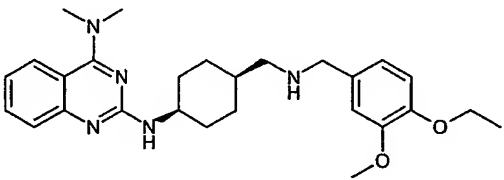
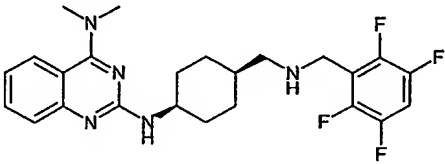
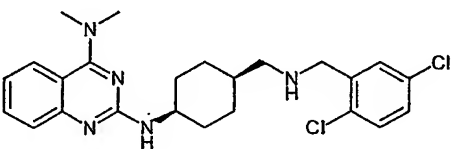
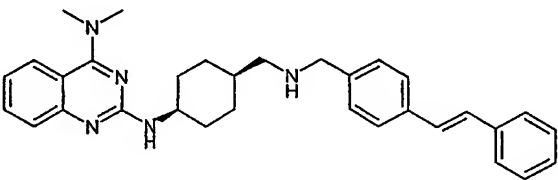
Example No.	Structure	APCI-MS
2237		420 (M + H)
2238		568 (M + H)
2239		428 (M + H)
2240		396 (M + H)
2241		420 (M + H)

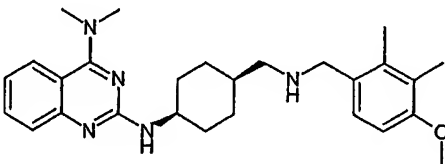
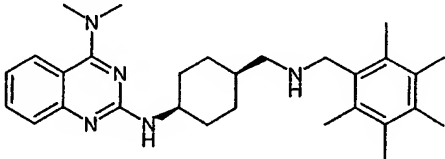
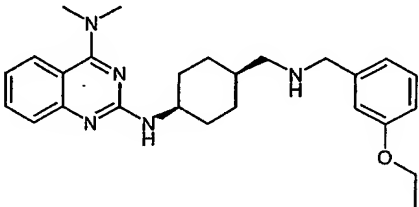
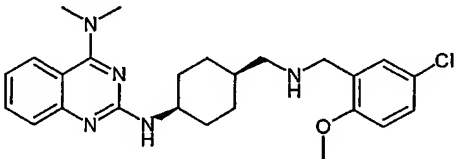
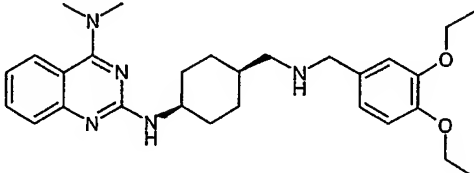
Example No.	Structure	APCI-MS
2242		468 (M + H)
2243		432 (M + H)
2244		468 (M + H)
2245		458 (M + H)
2246		423 (M + H)

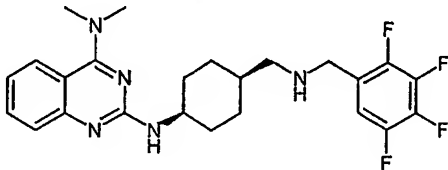
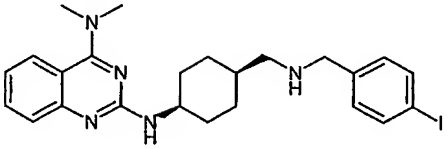
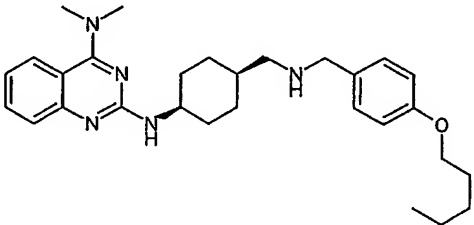
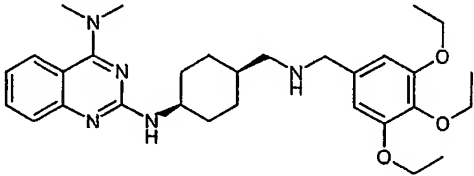
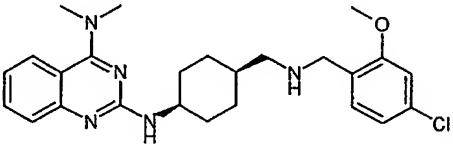
Example No.	Structure	APCI-MS
2247		420 (M + H)
2248		404 (M + H)
2249		448 (M + H)
2250		446 (M + H)
2251		540 (M + H)

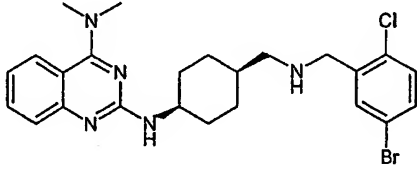
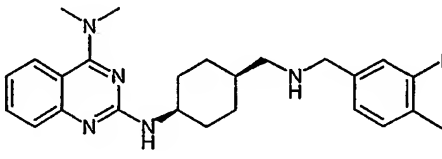
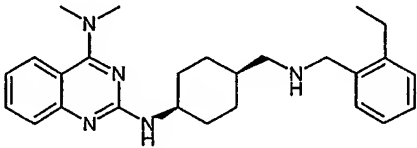
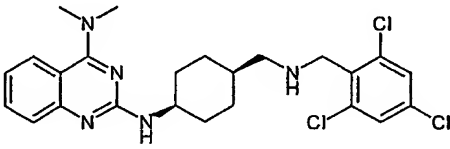
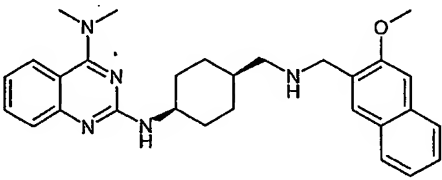
Example No.	Structure	APCI-MS
2252		470 (M + H)
2253		472 (M + H)
2254		479 (M + H)
2255		433 (M + H)
2256		458 (M + H)

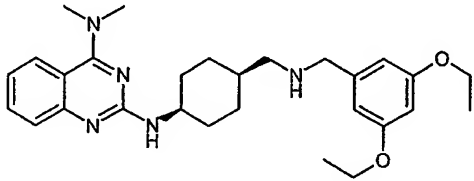
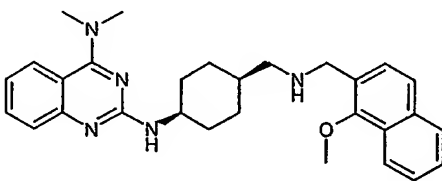
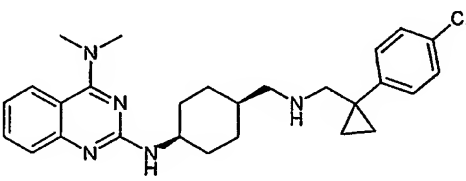
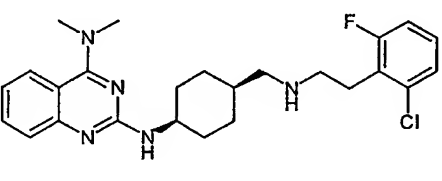
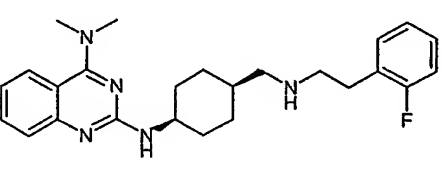
Example No.	Structure	APCI-MS
2257		515 (M + H)
2258		410 (M + H)
2259		394 (M + H)
2260		368 (M + H)
2261		372 (M + H)

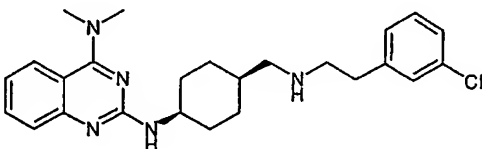
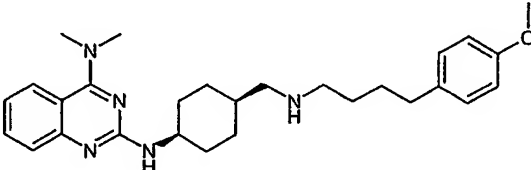
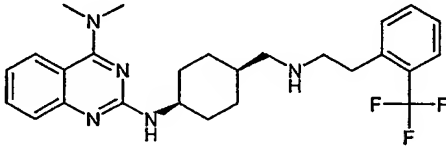
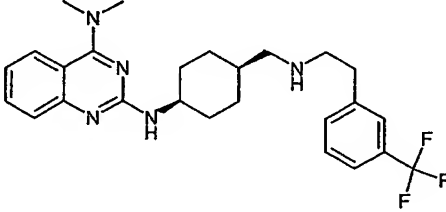
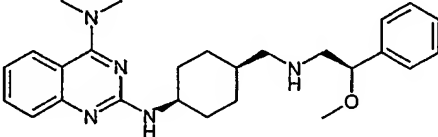
Example No.	Structure	APCI-MS
2262		397 (M + H)
2263		464 (M + H)
2264		462 (M + H)
2265		458 (M + H)
2266		492 (M + H)

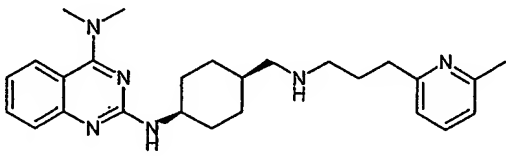
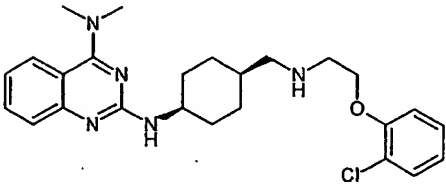
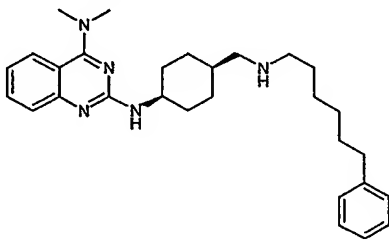
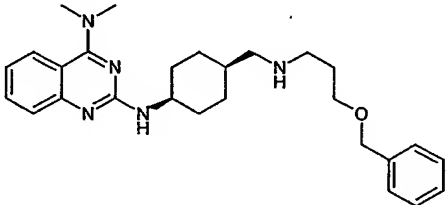
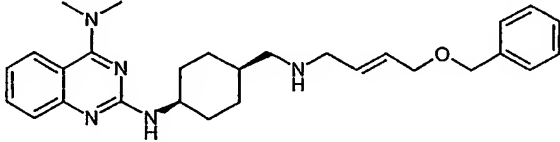
Example No.	Structure	APCI-MS
2267		448 (M + H)
2268		460 (M + H)
2269		434 (M + H)
2270		454 (M + H)
2271		478 (M + H)

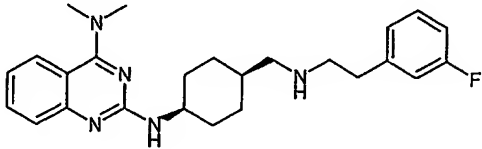
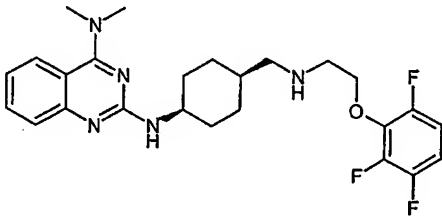
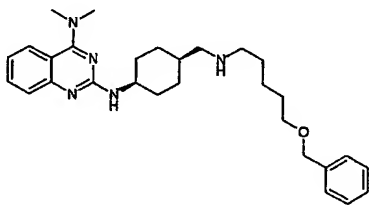
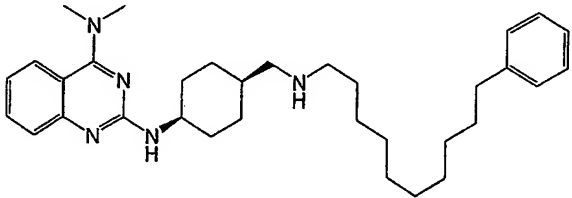
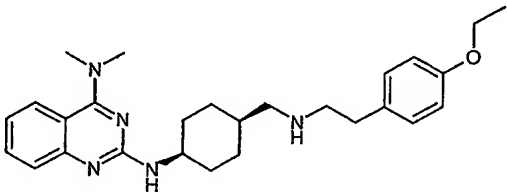
Example No.	Structure	APCI-MS
2272		462 (M + H)
2273		516 (M + H)
2274		476 (M + H)
2275		522 (M + H)
2276		454 (M + H)

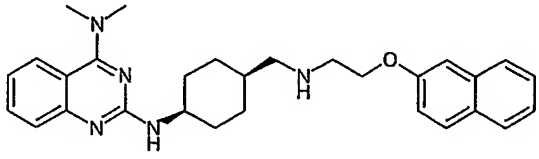
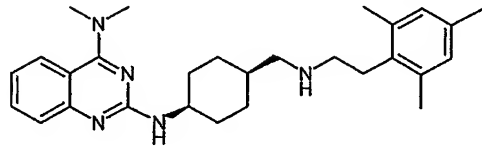
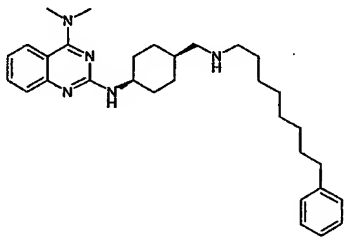
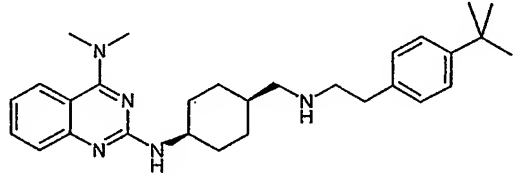
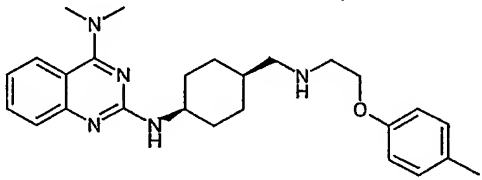
Example No.	Structure	APCI-MS
2277		502 (M + H)
2278		530 (M + H)
2279		418 (M + H)
2280		492 (M + H)
2281		470 (M + H)

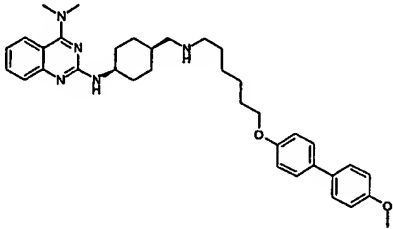
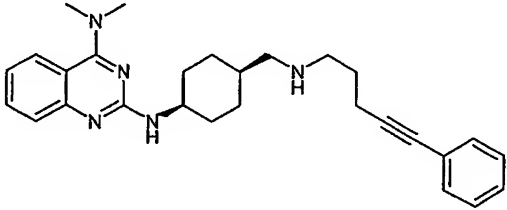
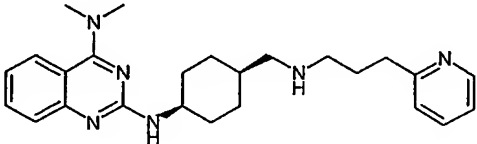
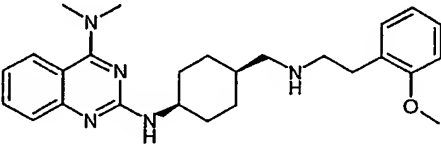
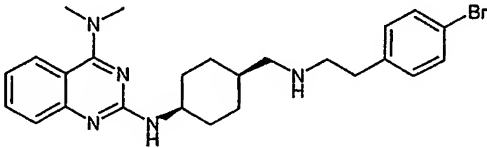
Example No.	Structure	APCI-MS
2282		478 (M + H)
2283		470 (M + H)
2284		464 (M + H)
2285		456 (M + H)
2286		422 (M + H)

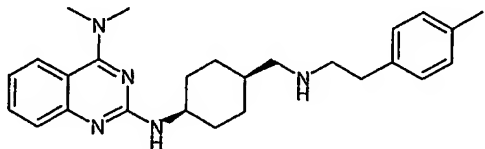
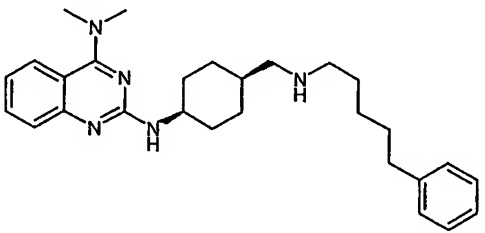
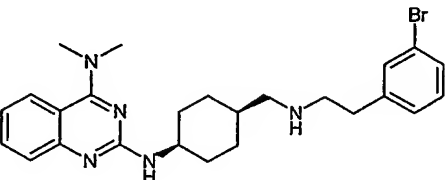
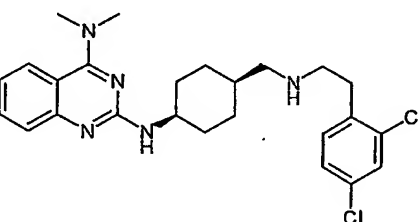
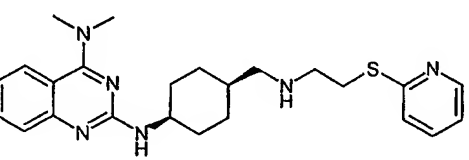
Example No.	Structure	APCI-MS
2287		438 (M + H)
2288		462 (M + H)
2289		472 (M + H)
2290		472 (M + H)
2291		434 (M + H)

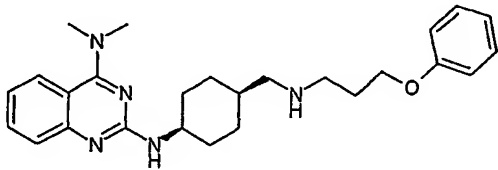
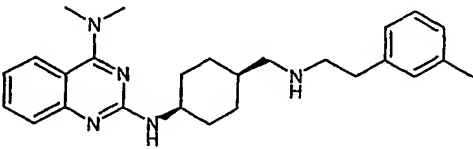
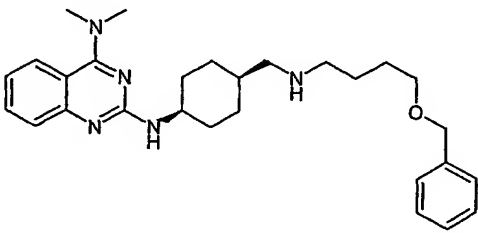
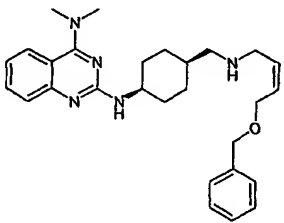
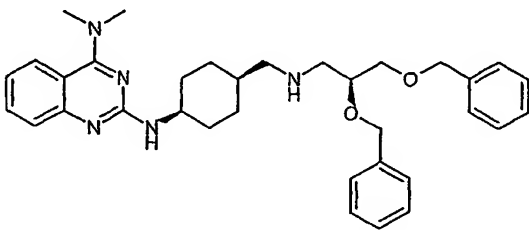
Example No.	Structure	APCI-MS
2292		433 (M + H)
2293		454 (M + H)
2294		460 (M + H)
2295		448 (M + H)
2296		460 (M + H)

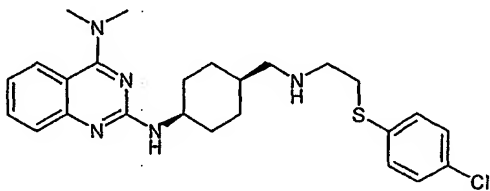
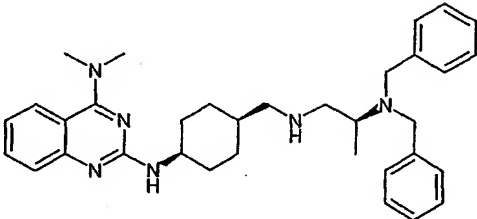
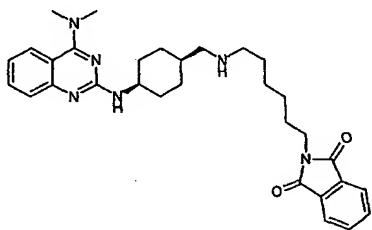
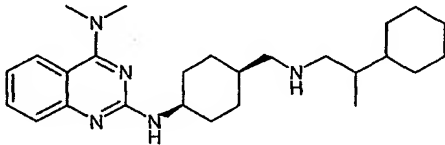
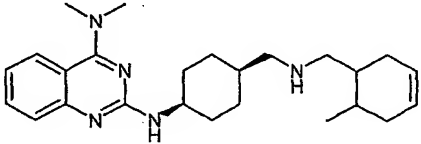
Example No.	Structure	APCI-MS
2297		422 (M + H)
2298		474 (M + H)
2299		476 (M + H)
2300		516 (M + H)
2301		448 (M + H)

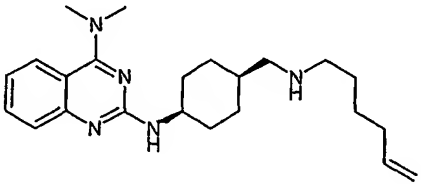
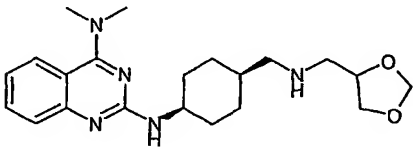
Example No.	Structure	APCI-MS
2302		470 (M + H)
2303		446 (M + H)
2304		488 (M + H)
2305		460 (M + H)
2306		434 (M + H)

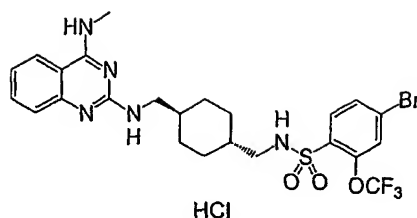
Example No.	Structure	APCI-MS
2307		582 (M + H)
2308		442 (M + H)
2309		419 (M + H)
2310		434 (M + H)
2311		482 (M + H)

Example No.	Structure	APCI-MS
2312		418 (M + H)
2313		446 (M + H)
2314		482 (M + H)
2315		472 (M + H)
2316		437 (M + H)

Example No.	Structure	APCI-MS
2317		434 (M + H)
2318		418 (M + H)
2319		462 (M + H)
2320		460 (M + H)
2321		554 (M + H)

Example No.	Structure	APCI-MS
2322		470 (M + H)
2323		537 (M + H)
2324		529 (M + H)
2325		424 (M + H)
2326		408 (M + H)

Example No.	Structure	APCI-MS
2327	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNC4CCCCC4C=C</chem>	382 (M + H)
2328	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNC4CCCC4COC5OCCO5</chem>	386 (M + H)

Example 2329

***trans*-4-Bromo-*N*-{4-[(4-methylamino-quinazolin-2-ylamino)-methyl]-cyclohexylmethyl}-2-trifluoromethoxy-benzenesulfonamide hydrochloride**

Step A: Synthesis of *trans*-4-[(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-cyclohexanecarboxylic acid.

To a solution of *trans*-4-aminomethyl-cyclohexanecarboxylic acid (3.14 g, 20 mmol) in THF (20 mL) and 1 M aqueous sodium hydroxide (42 mL) was added a solution of 4-bromo-2-trifluoromethoxy benzenesulfonyl chloride (6.9 g, 20.4 mmol) in THF (20 mL) and the mixture was stirred for 2 hr at ambient temperature. The resulting mixture was concentrated and 1 M aqueous HCl (45 mL) was added. The resulting precipitate was filtered, washed with water and hexanes to give *trans*-4-[(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-cyclohexanecarboxylic acid (7.18 g, 78%) as a white powder.

ESI MS *m/e* 460/462 $M + H^+$; 1H NMR (500 MHz, DMSO- d_6) δ 12.00 (brs, 1 H), 7.99 (brs, 1 H), 7.84-7.80 (m, 3 H), 2.72 (d, $J = 6.3$ Hz, 2 H), 2.10 (m, 1 H), 1.86 (m, 2 H), 1.71 (m, 2 H), 1.31 (m, 1 H), 1.23 (m, 2 H), 0.87 (m, 2 H).

Step B: Synthesis of *trans*-4-[(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-cyclohexanecarboxylic acid amide.

A solution of *trans*-4-[(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-cyclohexanecarboxylic acid (7.14 g, 15.5 mmol) and triethylamine (2.35 mL, 16.9 mmol) in THF (25 mL) was cooled to 0 °C. To the mixture was added ethyl chloroformate (1.62 mL, 17 mmol) in THF (5 mL) over 10 min. After stirring at 0 °C for 15 min, aqueous ammonia (27 mL) was added dropwise and the mixture was stirred at ambient temperature for 2 hr. The mixture was concentrated under reduced pressure and the concentrate was treated with water to give a solid. The solid was filtered and washed with water and hexanes to give *trans*-4-[(4-bromo-2-trifluoromethoxy-

benzenesulfonylamino)-methyl]-cyclohexanecarboxylic acid amide as a white solid (4.2 g, 59%).

ESI MS m/e 459/461 $M + H^+$; 1H NMR (500 MHz, DMSO- d_6) δ 7.98 (brs, 1 H), 7.84-7.80 (m, 3 H), 7.13 (s, 1 H), 6.62 (s, 1 H), 2.72 (d, $J = 6.5$ Hz, 2 H), 1.98 (m, 1 H), 1.70 (m, 4 H), 1.29 (m, 1 H), 1.23 (m, 2 H), 0.83 (m, 2 H).

Step C: Synthesis of *trans*-*N*-(4-aminomethyl-cyclohexylmethyl)-4-bromo-2-trifluoromethoxy-benzenesulfonamide.

To a solution of *trans*-4-[(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-cyclohexanecarboxylic acid amide (4.2 g, 9.2 mmol) in THF (40 mL) was added a solution of 1 M BH_3 in THF (32 mL, 32 mmol) over 40 min. The mixture was refluxed for 2 hr. After cooling to 0 °C, the mixture was quenched with water (7 mL). To the resulting mixture were added 4 M HCl in EtOAc (28 mL) and MeOH (28 mL) and the mixture was concentrated. To the residue was added MeOH (28 mL) and the mixture was once again concentrated. The resulting HCl-salt was recrystallized from Et_2O and subsequently neutralized with 1 M aqueous sodium hydroxide. The aqueous layer was extracted with CH_2Cl_2 (twice), the organic layers combined, dried over sodium sulfate, and concentrated under reduced pressure to give *trans*-*N*-(4-aminomethyl-cyclohexylmethyl)-4-bromo-2-trifluoromethoxy-benzenesulfonamide as a white solid (3.0 g, 74%).

ESI MS m/e 445/447 $M + H^+$; 1H NMR (500 MHz, DMSO- d_6) δ 7.84-7.79 (m, 3 H), 3.42 (brs, 2 H), 2.72 (d, $J = 6.8$ Hz, 2 H), 2.33 (d, $J = 6.5$ Hz, 2 H), 1.73 (m, 4 H), 1.27 (m, 1 H), 1.09 (m, 1 H), 0.80 (m, 4 H).

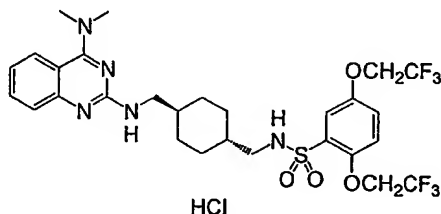
Step D: Synthesis of *trans*-4-Bromo-*N*-{4-[(4-methylamino-quinazolin-2-ylamino)-methyl]-cyclohexylmethyl}-2-trifluoromethoxy-benzenesulfonamide hydrochloride.

A mixture of (2-chloro-quinazolin-4-yl)-methylamine obtained in step A of example 50 (58 mg, 0.3 mmol) and *trans*-*N*-(4-aminomethyl-cyclohexylmethyl)-4-bromo-2-trifluoromethoxy-benzenesulfonamide amide (133 mg, 0.3 mmol) in 2-propanol (0.5 mL) was stirred at reflux for 24 hr. The mixture was cooled and the resulting white solid was collected by filtration and washed with 2-propanol to give *trans*-4-Bromo-*N*-{4-[(4-methylamino-quinazolin-2-ylamino)-methyl]-cyclohexylmethyl}-2-trifluoromethoxy-benzenesulfonamide hydrochloride as a white solid (121 mg, 67%).

ESI MS m/e 602/604 $M + H^+$; 1H NMR (500 MHz, DMSO- d_6) δ 12.61 (brs, 1 H), 9.70

(brs, 1 H), 8.26 (d, $J = 8.1$ Hz, 1 H), 8.15 (brs, 1 H), 8.02 (t, $J = 5.7$ Hz, 1 H), 7.84-7.74 (m, 4 H), 7.41 (m, 1 H), 3.32 (m, 2 H), 3.07 (d, $J = 3.5$ Hz, 3 H), 2.73 (t, $J = 6.2$ Hz, 2 H), 1.77 (m, 4 H), 1.53 (m, 1 H), 1.32 (m, 1 H), 0.96 (m, 2 H), 0.82 (m, 2 H).

Example 2330



trans-N-{4-[(4-Dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexylmethyl}-2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonamide hydrochloride

Step A: Synthesis of *trans*-4-{[2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonylamino]-methyl}-cyclohexanecarboxylic acid.

To a solution of *trans*-4-aminomethyl-cyclohexanecarboxylic acid (1.5 g, 10 mmol) in THF (10 mL) and 1 M aqueous sodium hydroxide (27 mL) was added a solution of 2,5-bis(2,2,2-trifluoroethoxy) benzenesulfonyl chloride (3.8 g, 10.25 mmol) in THF (10 mL) dropwise and the mixture was stirred at ambient temperature for 2 hr. The resulting mixture was concentrated and 1 M aqueous HCl (22.5 mL) was added. The resulting precipitate was filtered, washed with water and hexanes to give *trans*-4-{[2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonylamino]-methyl}-cyclohexanecarboxylic acid as a white powder (2.8 g, 57%).

ESI MS m/e 494 $M + H^+$; 1H NMR (500 MHz, DMSO- d_6) δ 7.36 (m, 3 H), 7.23 (brs, 1 H), 4.88 (m, 4 H), 2.73 (m, 2 H), 2.10 (m, 1 H), 1.87 (m, 2 H), 1.72 (m, 2 H), 1.30 (m, 1 H), 1.23 (m, 2 H), 0.87 (m, 2 H).

Step B: Synthesis of *trans*-4-{[2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonylamino]-methyl}-cyclohexanecarboxylic acid amide.

A solution of *trans*-4-{[2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonylamino]-methyl}-cyclohexanecarboxylic acid (2.78 g, 5.63 mmol) and triethylamine (1.9 mL,

13.6 mmol) in THF (25 mL) was cooled to 0 °C. To the mixture was added ethyl chloroformate (0.586 mL, 6.2 mmol) in THF (5 mL) over 10 min. After stirring at 0 °C for 15 min, 25% aqueous ammonia (10 mL) was added dropwise. The mixture was stirred at ambient temperature for 2 hr. The resulting mixture was concentrated under reduced pressure and the concentrate was diluted with water to give a solid. The solid was filtered and washed with water and hexanes to give *trans*-4-{[2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonylamino]-methyl}-cyclohexanecarboxylic acid amide as a white solid (2.7 g, 98%).

ESI MS m/e 493 $M + H^+$; 1H NMR (500 MHz, DMSO- d_6) δ 7.36 (m, 3 H), 7.23 (t, $J = 6.1$ Hz, 1 H), 7.13 (s, 1 H), 6.62 (s, 1 H), 4.88 (m, 4 H), 2.74 (t, $J = 6.4$ Hz, 2 H), 1.99 (m, 1 H), 1.75 (m, 4 H), 1.28 (m, 1 H), 1.23 (m, 2 H), 0.83 (m, 2 H).

Step C: Synthesis of *trans*-*N*-(4-aminomethyl-cyclohexylmethyl)-2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonamide.

To a solution of *trans*-4-{[2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonylamino]-methyl}-cyclohexanecarboxylic acid amide (2.7 g, 5.5 mmol) in THF (20 mL) was added a solution of 1 M BH_3 in THF (20 mL, 20 mmol) over 40 min. The mixture was stirred at reflux for 2 hr. After cooling to 0 °C, the mixture was quenched with water (7 mL). To the mixture were added 4 M HCl in EtOAc (28 mL) and MeOH (50 mL) and the mixture was concentrated. To the residue was added MeOH (50 mL) and the mixture was once again concentrated. The resulting HCl-salt was recrystallized from Et_2O and subsequently neutralized with 1 M aqueous sodium hydroxide. The aqueous layer was extracted with CH_2Cl_2 (twice), the combined organic layers were dried over sodium sulfate, and concentrated under reduced pressure to give *trans*-*N*-(4-aminomethyl-cyclohexylmethyl)-2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonamide as a white solid (1.5 g, 57%).

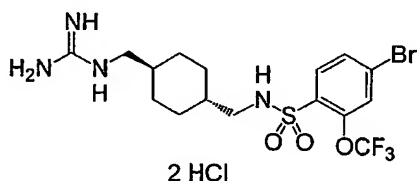
ESI MS m/e 479 $M + H^+$; 1H NMR (500 MHz, DMSO- d_6) δ 7.36-7.32 (m, 3 H), 6.62 (brs, 1 H), 4.88-4.78 (m, 4 H), 3.42 (b, 2 H), 2.73 (d, $J = 6.6$ Hz, 2 H), 2.34 (d, $J = 6.3$ Hz, 2 H), 1.73 (m, 4 H), 1.27 (m, 1 H), 1.10 (m, 1 H), 0.77 (m, 4 H).

Step D: Synthesis of *trans*-*N*-{4-[(4-Dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexylmethyl}-2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonamide hydrochloride.

A mixture of (2-chloro-quinazoline-4-yl)-dimethyl-amine obtained in step B of example 1 (41.4 mg, 0.2 mmol) and *trans*-*N*-(4-aminomethyl-cyclohexylmethyl)-2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonamide (95.6 mg, 0.2 mmol) in 2-propanol was stirred at reflux for 24 hr. The reaction mixture was concentrated and the residue was purified by column chromatography (silica gel) to give the product as a white foam. The product was dissolved in CH₂Cl₂ and treated with 1 M HCl in Et₂O. The mixture was concentrated to give *trans*-*N*-{4-[(4-Dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexylmethyl}-2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonamide hydrochloride as a white foam (101 mg, 78%).

ESI MS *m/e* 650 *M* + *H*⁺ ; ¹H NMR (500 MHz, DMSO-*d*₆) δ 8.16 (d, *J* = 8.2 Hz, 1 H), 8.00 (brs, 1 H), 7.78 (t, *J* = 7.9, 1 H), 7.44 (brs, 1 H), 7.34 (m, 4 H), 7.24 (t, *J* = 5.9 Hz, 1 H), 4.88 (m, 4 H), 3.32 (s, 6 H), 3.29 (m, 2 H), 2.75 (t, *J* = 6.2 Hz, 2 H), 1.74 (m, 4 H), 1.52 (m, 1 H), 1.32 (m, 1 H), 0.94 (m, 2 H), 0.83 (m, 2 H).

Example 2331



***trans*-4-Bromo-*N*-(4-guanidinomethyl-cyclohexylmethyl)-2-trifluoromethoxy-benzenesulfonamide dihydrochloride**

Step A: Synthesis of *trans*-[({4-[(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-cyclohexylmethyl}-amino)-*tert*-butoxycarbonylamino-methyl]-carbamic acid *tert*-butyl ester.

To a solution of *trans*-*N*-(4-aminomethyl-cyclohexylmethyl)-4-bromo-2-trifluoromethoxy-benzenesulfonamide obtain in step C of example 2329 (45 mg, 0.1 mmol) and triethylamine (14 μL, 0.1 mmol) in CH₂Cl₂ (5 mL) was added (*tert*-butoxycarbonylamino-trifluoromethanesulfonylimino-methyl)-carbamic acid *tert*-butyl ester (39.1 mg, 0.1 mmol). The reaction mixture was stirred at ambient temperature for 2 hr and concentrated. The residue was purified by column chromatography (silica gel,

CH_2Cl_2 to 10% MeOH in CH_2Cl_2) to give *trans*-[({4-[(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-

cyclohexylmethyl}-amino)-*tert*-butoxycarbonylamino-methyl]-carbamic acid

tert-butyl ester as a white solid (63 mg, 92%).

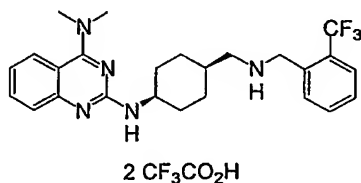
ESI MS m/e 687/689 $M + H^+$; ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 11.45 (s, 1 H), 8.22 (t, $J = 5.6$ Hz, 1 H), 7.97 (t, $J = 5.6$ Hz, 1 H), 7.99-7.79 (m, 3 H), 3.13 (t, $J = 6.4$ Hz, 2 H), 2.72 (t, $J = 6$ Hz, 2 H), 1.70 (m, 4 H), 1.46 (s, 9 H), 1.38 (s, 9 H), 1.31 (m, 2 H), 0.83 (m, 4 H).

Step B: Synthesis of *trans*-4-bromo-*N*-(4-guanidinomethyl-cyclohexylmethyl)-2-trifluoromethoxy-benzenesulfonamide dihydrochloride.

A solution of *trans*-[({4-[(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-cyclohexylmethyl}-amino)-*tert*-butoxycarbonylamino-methyl]-carbamic acid *tert*-butyl ester (53 mg, 0.077 mmol) in 50% TFA in CH_2Cl_2 (2 mL) was stirred at ambient temperature for 3 hr and the reaction mixture was concentrated. To the residue was added a solution of 1 M HCl in Et_2O (0.5 mL) and the mixture was concentrated to give *trans*-4-Bromo-*N*-(4-guanidinomethyl-cyclohexylmethyl)-2-trifluoromethoxy-benzenesulfonamide dihydrochloride as a white solid (29 mg, 68%).

ESI MS m/e 487/489 $M + H^+$; ^1H NMR (500 MHz, $\text{DMSO}-d_6$) δ 8.01 (t, $J = 5.5$ Hz, 1 H), 7.84 (m, 3 H), 7.68 (m, 1 H), 7.30 (m, 2 H), 6.85 (m, 2 H), 2.94 (t, $J = 6.1$ Hz, 2 H), 2.74 (t, $J = 6.1$ Hz, 2 H), 1.71 (m, 2 H), 1.31 (m, 4 H), 0.86 (m, 4 H).

Example 2332



cis- N^4,N^4 -Dimethyl- N^2 -{4-[(2-trifluoromethyl-benzylamino)-methyl]-cyclohexyl}-quinazoline-2,4-diamine ditrifluoro-acetic acid

Step A: Synthesis of *cis*-4-*tert*-butoxycarbonylamino-cyclohexanecarboxylic acid.

To a solution of *cis*-4-amino-cyclohexanecarboxylic acid (50 g, 350 mmol) in THF

(200 mL) and 1 M aqueous sodium hydroxide (380 mL, 380 mmol) was added (Boc)₂O (83.5 g, 360 mmol). The reaction mixture was stirred at ambient temperature for 2 hr and concentrated. The residue was cooled to 0 °C followed by acidification with 1 M HCl (pH = 3). The resulting white solid was filtered, washed with water and hexanes to give *cis*-4-*tert*-butoxycarbonylamino-cyclohexanecarboxylic acid (71g, 83%) as a white solid. ESI MS *m/e* 244 *M* + *H*⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.00 (brs, 1 H), 6.74 (d, *J* = 4.25, 1 H), 3.30 (brs, 1 H), 2.35 (m, 1 H), 1.87 (m, 2 H), 1.55-1.37 (m, 15 H).

Step B: Synthesis of *cis*-(4-carbamoyl-cyclohexyl)-carbamic acid *tert*-butyl ester.

To a solution cooled at 0°C of *cis*-4-*tert*-butoxycarbonylamino-cyclohexanecarboxylic acid (68.0 g, 280 mmol) and triethylamine (31.1 g, 307 mmol) in THF (300 mL) was added ethyl chloroformate (29.3 mL, 308 mmol) dropwise. After stirring at 0 °C for 30 min, 25% aqueous ammonia (168 mL) was added dropwise. The reaction mixture was stirred at ambient temperature for 2 hr and concentrated. The residue was extracted with EtOAc (three times). The combined organic layer was washed with saturated aqueous NaHCO₃, 1 M HCl, brine, and water, dried over Na₂SO₄, filtered, and concentrated to give *cis*-(4-carbamoyl-cyclohexyl)-carbamic acid *tert*-butyl ester (62.0 g, 88%) as a white solid.

ESI MS *m/e* 243 *M* + *H*⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.10 (brs, 1 H), 6.69 (b, 2 H), 3.41 (brs, 1 H), 2.14 (m, 1 H), 1.79 (m, 2 H), 1.59 (m, 2 H), 1.45-1.37 (m, 13 H).

Step C: Synthesis of *cis*-4-amino-cyclohexanecarboxylic acid amide hydrochloride.

To a solution of *cis*-(4-carbamoyl-cyclohexyl)-carbamic acid *tert*-butyl ester (62 g, 256 mmol) in CH₂Cl₂ (250 mL) was added TFA (250 mL) and the mixture was stirred at ambient temperature for 1 hr. The mixture was concentrated and 2 M HCl in Et₂O (150 mL) was added to give a white precipitate. The mixture was concentrated to give *cis*-4-amino-cyclohexanecarboxylic acid amide hydrochloride (45 g, 98%) as a white solid.

ESI MS *m/e* 143 *M* + *H*⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.08 (m, 3 H), 7.28 (s, 1 H), 6.78 (s, 1 H), 3.10 (m, 1 H), 2.24 (m, 1 H), 1.90 (m, 2 H), 1.66 (m, 4 H), 1.50 (m, 2 H).

Step D: Synthesis of *cis*-4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexanecarboxylic acid amide.

A solution of (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B of

example 1 (31.05 g, 150 mmol) and *cis*-4-amino-cyclohexanecarboxylic acid amide hydrochloride (26.7 g, 150 mmol) in pyridine (150 mL) was stirred at reflux for overnight. The reaction mixture was concentrated and residue was dissolve in CH₂Cl₂. The organic layer was washed with saturated aqueous NaHCO₃ and the aqueous layer was extracted with CH₂Cl₂. The organic layer was dried over Na₂SO₄, filtered and concentrated. The residue was purified by column chromatography (silica gel, 2% to 10% 2 M NH₃/MeOH in CH₂Cl₂) to give a slightly brown solid and the solid was recrystallized from CH₂Cl₂ to give *cis*-4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexanecarboxylic acid amide (20.6 g, 44%) as yellow crystals.

ESI MS *m/e* 314 M + H⁺; ¹H NMR (400 MHz, DMSO-d₆) δ 8.19 (brs, 1 H), 8.15 (d, *J* = 8.4 Hz, 1 H), 7.77 (t, *J* = 8.0 Hz, 1 H), 7.42 (d, *J* = 7.2 Hz, 1 H), 7.35 (t, *J* = 8.4 Hz, 1 H), 7.21 (s, 1 H), 6.74 (s, 1 H), 4.12 (m, 1 H), 3.46 (m, 6 H), 2.24 (m, 1 H), 1.79-1.61 (m, 8 H).

Step E: Synthesis of *cis*-N²-(4-aminomethyl-cyclohexyl)-N⁴,N⁴-dimethyl-quinazoline-2,4-diamine.

To a solution of *cis*-4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexanecarboxylic acid amide (18.78 g, 60 mmol) in THF (200 mL) was added a solution of 1 M BH₃ in THF (300 mL, 300 mmol). The mixture was stirred at reflux for 2 hr. After cooling the reaction mixture to 0 °C, 4 M HCl in EtOAc (100 mL) and MeOH (200 mL) were added. The mixture was concentrated. The mixture was treated with 1 M aqueous sodium hydroxide and the aqueous layer was extracted with CH₂Cl₂. The organic layer was dried over sodium sulfate, concentrated, and purified by column chromatography (silica gel, 10% 2 M NH₃/MeOH in CH₂Cl₂) to give *cis*-N²-(4-aminomethyl-cyclohexyl)-N⁴,N⁴-dimethyl-quinazoline-2,4-diamine as a white solid (10.6 g, 59%).

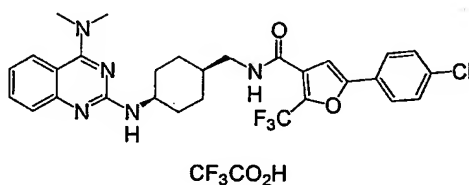
ESI MS *m/e* 300 M + H⁺; ¹H NMR (400 MHz, DMSO-d₆) δ 7.84 (d, *J* = 8.4 Hz, 1 H), 7.46 (t, *J* = 6.8 Hz, 1 H), 7.26 (d, *J* = 8.4 Hz, 1 H), 6.99 (t, *J* = 6.8 Hz, 1 H), 6.28 (brs, 1 H), 4.02 (m, 1 H), 3.19 (m, 6 H), 2.47 (d, *J* = 6.8 Hz, 2 H), 2.73 (m 2 H), 1.68-1.33 (m, 9 H).

Step F: Synthesis of *cis*-N⁴,N⁴-dimethyl-N²-{4-[(2-trifluoromethyl-benzylamino)-methyl]-cyclohexyl}-quinazoline-2,4-diamine ditrifluoro-acetic acid.

A solution of *cis*-*N*²-(4-aminomethyl-cyclohexyl)-*N*⁴,*N*⁴-dimethyl-quinazoline-2,4-diamine (33 mg, 0.11 mmol) and 2-trifluoromethyl benzaldehyde (17.41 mg, 0.1 mmol) in MeOH (1 mL) was stirred at ambient temperature for 3 hr. To the mixture was added NaBH(OAc)₃ (85 mg, 0.4 mmol) and the mixture was stirred at ambient temperature for overnight. This resulting mixture was quenched with 50% DMSO in water (2 mL) and the solution was purified by preparative HPLC. The pure fractions were combined and lyophilized to give *cis*-*N*⁴,*N*⁴-dimethyl-*N*²-{4-[(2-trifluoromethyl-benzylamino)-methyl]-cyclohexyl}-quinazoline-2,4-diamine ditrifluoro-acetic acid (41.4 mg, 60%) as a white solid.

ESI MS *m/e* 458 *M* + *H*⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 13.12 (brs, 1 H), 8.94 (b, 2 H), 8.65 (d, *J* = 6.8 Hz, 1 H), 8.16 (d, *J* = 8.8 Hz, 1 H), 7.77-7.66 (m, 5 H), 7.41 (d, *J* = 8.4 Hz, 1 H), 7.35 (t, *J* = 8 Hz, 1 H), 4.22 (s, 2 H), 4.17 (m, 1 H), 3.46 (b, 6 H), 2.94 (m, 2 H), 1.87-1.44 (m, 9 H).

Example 2333



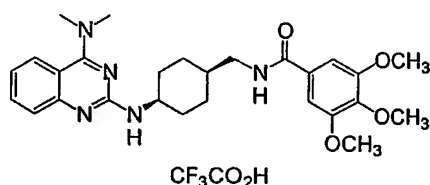
cis-5-(4-Chloro-phenyl)-2-trifluoromethyl-furan-3-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexylmethyl]-amide trifluoro-acetic acid

Step A: Synthesis of *cis*-5-(4-chloro-phenyl)-2-trifluoromethyl-furan-3-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexylmethyl]-amide trifluoro-acetic acid.

A solution of *cis*-*N*²-(4-aminomethyl-cyclohexyl)-*N*⁴,*N*⁴-dimethyl-quinazoline-2,4-diamine obtained in step E of example 2332 (30 mg, 0.1 mmol), 5-(4-chloro-phenyl)-2-trifluoromethyl-furan-3-acid chloride (37 mg, 0.12 mmol), and pyridine (12 μL, 0.15 mmol) in DMF (0.5 mL) was stirred at ambient temperature for overnight. The resulting mixture was diluted with DMSO (0.8 mL) and the mixture was purified by preparative

HPLC. The pure fractions were combined and lyophilized to give *cis*-5-(4-chloro-phenyl)-2-trifluoromethyl-furan-3-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexylmethyl]-amide trifluoro-acetic acid (17.5 mg, 26%) as a white solid. ESI MS m/e 572 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 12.30 (brs, 1 H), 8.65 (t, J = 6.8 Hz, 1 H), 8.19 (brs, 1 H), 8.14 (d, J = 8.0 Hz, 1 H), 7.83-7.30 (m, 8 H), 4.1 (m, 1 H), 3.46 (b, 6 H), 3.09 (m, 2 H), 1.77-1.38 (m, 9 H).

Example 2334



cis-N-[4-(4-Dimethylamino-quinazolin-2-ylamino)-cyclohexylmethyl]-3,4,5-trimethoxy-benzamide trifluoro-acetic acid

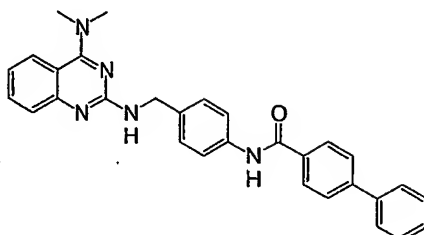
Step A: Synthesis of *cis*-N-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexylmethyl]-3,4,5-trimethoxy-benzamide trifluoro-acetic acid.

To HOBT-6-carboxamidomethyl polystyrene 200-400 mesh (77 mg, 0.1 mmol) were added a solution of 0.3 M PyBroP in DMF (1 mL, 0.3 mmol), 3,4,5-trimethoxybenzoic acid (63 mg, 0.3 mmol), and diisopropylethylamine (85 μ L, 0.5 mmol). The mixture was stirred at ambient temperature for 5 hr. The resin was washed with DMF (3 times), CH_2Cl_2 (3 times), MeOH (3 times), CH_2Cl_2 (2 times), and DMF (2 times). To the resin was added *cis*-N²-(4-aminomethyl-cyclohexyl)-N⁴,N⁴-dimethyl-quinazoline-2,4-diamine obtained in step E of example 2332 (28 mg, 0.09 mmol) in DMF (0.5 mL) and the mixture was stirred at ambient temperature for overnight. The resin was filtered and washed with 0.5 mL DMSO (2 times). The combined filtrates were purified by preparative HPLC. The pure fractions were combined and lyophilized to give *cis* N-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexylmethyl]-3,4,5-trimethoxy-benzamide trifluoro-acetic acid (7.4 mg, 12%) as a white solid.

ESI MS m/e 494 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 12.25 (brs, 1 H), 8.45 (t, J = 5.6 Hz, 1 H), 8.17 (brs, 1 H), 8.14 (d, J = 8.0 Hz, 1 H), 7.76 (t, J = 8.4 Hz, 1 H), 7.42 (d, J

= 7.2 Hz, 1 H), 7.34 (t, J = 7.6 Hz, 1 H), 7.15 (s, 2 H), 4.13 (m, 1 H), 3.44 (s, 3 H), 3.39 (s, 3 H), 3.20 (m, 2 H), 1.77-1.37 (m, 9 H).

Example 2335



Biphenyl-4-carboxylic acid {4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-phenyl}-amide

Step A: Synthesis of (4-amino-benzyl)-carbamic acid *tert*-butyl ester.

A solution of 4-aminomethyl-phenylamine (12.2 g, 100 mmol) and (Boc)₂O (21.8 g, 100 mmol) in CH₂Cl₂ (100 mL) was stirred at ambient temperature for overnight. The mixture was concentrated and the residue was purified by column chromatography (silica gel, CH₂Cl₂ to 10% MeOH in CH₂Cl₂) to give (4-amino-benzyl)-carbamic acid *tert*-butyl ester (11.6 g, 52%) as a slightly yellow solid.

ESI MS m/e 223 M + H⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.27 (t, J = 6.0 Hz, 1 H), 6.86 (d, J = 8.0 Hz, 2 H), 6.47 (d, J = 6.4 Hz, 2 H), 4.89 (s, 2 H), 3.91 (d, J = 6.0 Hz, 2 H), 1.39 (s, 9 H).

Step B: Synthesis of biphenyl-4-carboxylic acid (4-aminomethyl-phenyl)-amide hydrochloride.

To a solution of (4-amino-benzyl)-carbamic acid *tert*-butyl ester (1.11 g, 5 mmol), biphenyl carboxylic acid (0.99 g, 5 mmol), EDC (1.2 g, 6.25 mmol), and HOAt (0.82 g, 6 mmol) in CH₂Cl₂ (10 mL) was added triethylamine (pH = 10) and the mixture was stirred at ambient temperature for overnight. The organic layer was washed with saturated aqueous NaHCO₃, 1 M aqueous HCl, water, dried over Na₂SO₄, filtered, and concentrated. The residue was dissolved in 50% TFA in CH₂Cl₂ (10 mL) and the mixture was stirred at ambient temperature. After 30 minutes, the mixture was concentrated and diluted with 1 M HCl in Et₂O (5 mL). The mixture was concentrated to give biphenyl-4-carboxylic acid (4-aminomethyl-phenyl)-amide hydrochloride (828 mg, 49%).

ESI MS m/e 303 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 10.40 (s, 1 H), 8.34 (b, 3 H), 8.07 (d, $J = 8.0$ Hz, 2 H), 7.83-7.73 (m, 6 H), 7.51-7.38 (m, 5 H), 4.0 (q, $J = 5.6$ Hz, 2 H).

Step C: Synthesis of biphenyl-4-carboxylic acid {4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-phenyl}-amide.

A mixture of (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B of example 1 (42 mg, 0.2 mmol) and biphenyl-4-carboxylic acid (4-aminomethyl-phenyl)-amide hydrochloride (49 mg, 0.14 mmol) in 2-propanol (1 mL) and triethylamine (200 μ L) was stirred at reflux for 2 days. The resulting mixture was concentrated and purified by column chromatography (silica gel, CH_2Cl_2 to 10% 2 M $NH_3/MeOH$ in CH_2Cl_2) to give biphenyl-4-carboxylic acid {4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-phenyl}-amide (10 mg, 15%) as a white solid.

ESI MS m/e 474 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 10.19 (s, 1 H), 8.02 (d, $J = 7.2$ Hz, 2 H), 7.86 (d, $J = 8.4$ Hz, 1 H), 7.80 (d, $J = 8.4$ Hz, 2 H), 7.73 (d, $J = 7.2$ Hz, 2 H), 7.68 (d, $J = 7.6$ Hz, 2 H), 7.50-7.15 (m, 8 H), 7.01 (t, $J = 8.4$ Hz, 1 H), 4.51 (d, $J = 6.4$ Hz, 2 H), 3.30 (s, 3 H), 3.2 (s, 3 H).

Example 2336



cis- N^2 -{4-[2-(4-Bromo-2-trifluoromethoxy-benzylamino)-ethyl]-cyclohexyl}- N^4,N^4 -dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid

Step A: Synthesis of *cis*-[4-(2-benzoyloxycarbonylamino-ethyl)-cyclohexyl]-carbamic acid *tert*-butyl ester.

To a solution of *cis*-[4-(2-amino-ethyl)-cyclohexyl]-carbamic acid *tert*-butyl ester (4.84 g, 20 mmol) in CH_2Cl_2 (50 mL) and triethylamine (3.06 mL, 22 mmol) was added benzyl chloroformate (3.13 mL, 22 mmol) and the mixture was stirred for 4 hr. The resulting mixture was washed with water, 1 M aqueous HCl, dried over Na_2SO_4 , filtered and concentrated. The residue was purified by column chromatography (silica gel,

CH₂Cl₂ to 10% MeOH in CH₂Cl₂) to give *cis*-[4-(2-benzyloxycarbonylamino-ethyl)-cyclohexyl]-carbamic acid *tert*-butyl ester (5.46 g, 73%) as a colorless oil.

ESI MS *m/e* 377 *M* + *H*⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.36-7.24 (m, 5 H), 7.19 (t, *J* = 5.6 Hz, 1 H), 6.76 (d, *J* = 6.8 Hz, 1 H), 4.91 (s, 2 H), 3.40 (m, 1 H), 2.99 (m, 2 H), 1.44-1.33 (m, 20H).

Step B: Synthesis of *cis*-[2-(4-amino-cyclohexyl)-ethyl]-carbamic acid benzyl ester.

A solution of *cis*-[4-(2-benzyloxycarbonylamino-ethyl)-cyclohexyl]-carbamic acid *tert*-butyl ester (5.26 g, 14 mmol) in 50% TFA in CH₂Cl₂ (60 mL) was stirred at ambient temperature for 1 hr. The mixture was concentrated and the residue was diluted with saturated aqueous NaHCO₃. The aqueous layer was extracted with CH₂Cl₂ (three times). The organic layer was dried over Na₂SO₄ and concentrated to give *cis*-[2-(4-amino-cyclohexyl)-ethyl]-carbamic acid benzyl ester (3.5 g, 91%) as a colorless oil.

ESI MS *m/e* 277 *M* + *H*⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.72 (b, 2 H), 7.34-7.27 (m, 5 H), 7.21 (t, *J* = 5.2 Hz, 1 H), 4.97 (s, 2 H), 3.14 (m, 1 H), 2.99 (q, *J* = 6.4 Hz, 2 H), 1.58-1.34 (m, 11 H).

Step C: Synthesis of *cis*-[2-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-ethyl]-carbamic acid benzyl ester.

A mixture of (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B of example 1 (2.45 g, 10.2 mmol) and *cis*-[2-(4-amino-cyclohexyl)-ethyl]-carbamic acid benzyl ester (3.3 g, 10.2 mmol) and triethylamine (1.65 mL, 10.2 mmol) in 2-propanol (15 mL) was heated at 170 °C for 45 min using a Smith Microwave Synthesizer. The mixture was concentrated and the residue was purified by column chromatography (silica gel, CH₂Cl₂ to 10% 2 M NH₃/MeOH in CH₂Cl₂) to give *cis*-[2-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-ethyl]-carbamic acid benzyl ester (4.48g, 85%) as a yellow oil.

ESI MS *m/e* 448 *M* + *H*⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.07-7.20 (m, 11 H), 4.98 (s, 2 H), 4.08 (m, 1 H), 3.39 (b, 6 H), 3.04 (m, 2 H), 1.7-1.3 (m, 11 H).

Step D: Synthesis of *cis*-*N*²-[4-(2-amino-ethyl)-cyclohexyl]-*N*²,*N*²-dimethyl-quinazoline-2,4-diamine.

To a solution of *cis*-[2-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-

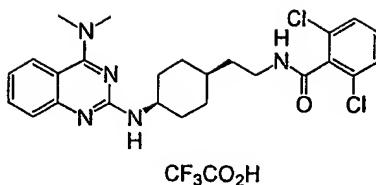
ethyl}-carbamic acid benzyl ester (4.47 g, 10 mmol) in EtOH (20 mL) was added 1,4-cyclohexadiene (20 mL) and 200 mg of 10% Pd/C. The reaction mixture was stirred at ambient temperature for 18 hr, filtered through pad of celite, and concentrated. The residue was purified by column chromatography (silica gel, 5% to 15% 2 M NH₃/MeOH in CH₂Cl₂) to give *cis*-N²-[4-(2-amino-ethyl)-cyclohexyl]-N',N'-dimethyl-quinazoline-2,4-diamine (2.41 g, 77%) as a yellow oil.

ESI MS m/e 314 M + H⁺; ¹H NMR (400 MHz, DMSO-d₆) δ 7.82 (d, *J* = 8.0 Hz, 1 H), 7.44 (t, *J* = 6.8 Hz, 1 H), 7.27 (d, *J* = 8.0 Hz, 1 H), 6.97 (t, *J* = 6.8 Hz, 1 H), 6.31 (brs, 1 H), 3.97 (m, 1 H), 3.37 (b, 2 H), 3.17 (s, 3), 3.14 (s, 3 H), 2.62 (t, *J* = 7.6 Hz, 2 H), 1.68-1.31 (m, 11 H).

Step E: Synthesis of *cis*-N²-{4-[2-(4-bromo-2-trifluoromethoxy-benzylamino)-ethyl]-cyclohexyl}-N',N'-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid.

A solution of *cis*-N²-[4-(2-amino-ethyl)-cyclohexyl]-N',N'-dimethyl-quinazoline-2,4-diamine (31.4 mg, 0.1 mmol) and 4-bromo-2-trifluoromethoxy benzaldehyde (26.9 mg, 0.1 mmol) in MeOH (1 mL) was stirred at ambient temperature. After 3 hr, NaBH(OAc)₃ (85 mg, 0.4 mmol) was added and the resulting mixture was stirred at ambient temperature for overnight. The reaction mixture was quenched with 50% DMSO in water (2 mL). The mixture was concentrated and purified by preparative HPLC. The pure fractions were combined and lyophilized to give *cis*-N²-{4-[2-(4-bromo-2-trifluoromethoxy-benzylamino)-ethyl]-cyclohexyl}-N',N'-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid (32.2 mg, 41%) as a white solid.

ESI MS m/e 566/568 M + H⁺; ¹H NMR (400 MHz, DMSO-d₆) δ 12.76 (brs, 1 H), 8.81 (b, 2 H), 8.43 (m, 1 H), 8.09 (d, *J* = 8.4 Hz, 1 H), 7.71-7.56 (m, 4 H), 7.35 (d, *J* = 8.0 Hz, 1 H), 7.29 (t, *J* = 8.0 Hz, 1 H), 4.15 (m, 3 H), 3.39 (m, 6 H), 2.97 (m, 2 H), 1.67-1.30 (m, 11 H).

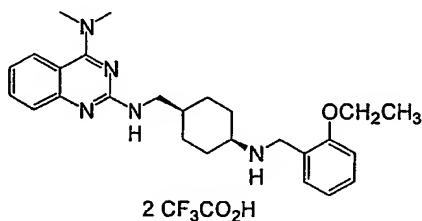
Example 2337

***cis*-2,6-Dichloro-*N*-{2-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-ethyl}-benzamide trifluoro-acetic acid**

Step A: Synthesis of *cis*-2,6-dichloro-*N*-{2-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-ethyl}-benzamide trifluoro-acetic acid.

To a solution of *cis*-*N*²-[4-(2-amino-ethyl)-cyclohexyl]-*N*¹,*N*¹-dimethyl-quinazoline-2,4-diamine (31.4 mg, 0.1 mmol) and 2,6-dichlorobenzoyl chloride (20.7 mg, 0.1 mmol) in DMF (0.5 mL) was added triethylamine (20 μ L, 0.14 mmol). After stirring the mixture at ambient temperature for 6 hr, DMSO (0.5 mL) was added and the mixture was purified by preparative HPLC. The pure fractions were combined and lyophilized to give *cis*-2,6-dichloro-*N*-{2-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-ethyl}-benzamide trifluoro-acetic acid (17.6 mg, 29%) as a white solid.

ESI MS m/e 486 $M + H^+$; ¹H NMR (400 MHz, DMSO- d_6) δ 11.93 (brs, 1 H), 8.26 (t, J = 5.2 Hz, 1 H), 8.14 (d, J = 8.0 Hz, 1 H), 7.95 (brs, 1 H), 7.76 (t, J = 8.4 Hz, 1 H), 7.52-7.31 (m, 5 H), 4.15 (m, 1 H), 3.45 (b, 6 H), 3.29 (m, 2 H), 1.76-1.31 (m, 11 H).

Example 2338

***cis*-*N*²-[4-(2-Ethoxy-benzylamino)-cyclohexylmethyl]-*N*¹,*N*¹-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid**

Step A: Synthesis of *cis*-(4-aminomethyl-cyclohexyl)-carbamic acid tert-butyl ester.

To a solution of *cis*-(4-carbamoyl-cyclohexyl)-carbamic acid *tert*-butyl ester obtained in step B of example 2332 (9.68 g, 40 mmol) in THF (100 mL) was added a solution of 1 M BH₃ in THF (80 mL, 80 mmol) over 30 min. The mixture was stirred at reflux for 2 hr. After cooling the reaction mixture to ambient temperature, 1 M aqueous sodium hydroxide was carefully added. The solvents were removed under reduced pressure and the aqueous layer was extracted with CH₂Cl₂ (twice). The organic layer was dried over sodium sulfate and concentrated under reduced pressure to give *cis*-(4-aminomethyl-cyclohexyl)-carbamic acid *tert*-butyl ester as colorless oil (5.16 g, 57%).

ESI MS *m/e* 229 M + H⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 6.67 (d, *J* = 6.8 Hz, 1 H), 3.43 (m, 1 H), 2.41 (d, *J* = 6.4 Hz, 2 H) 1.49-1.22 (m, 18 H).

Step B: Synthesis of *cis*-{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexyl}-carbamic acid *tert*-butyl ester.

A mixture of *cis*-(4-aminomethyl-cyclohexyl)-carbamic acid *tert*-butyl ester (1.14 g, 5 mmol), (2-chloro-quinazoline-4-yl)-dimethyl-amine obtained in step B of example 1 (1.035 g, 5 mmol), and triethylamine (1.5 mL, 11 mmol) in 2-propanol (2.5 mL) was heated at 170 °C for 35 min using a Smith Microwave Synthesizer. The mixture was concentrated and the residue was purified by column chromatography (silica gel, CH₂Cl₂ to 10% 2 M NH₃/MeOH in CH₂Cl₂) to give *cis*-{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexyl}-carbamic acid *tert*-butyl ester (1.28 g, 80%) as a white solid.

ESI MS *m/e* 400 M + H⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.04-7.06 (m, 4 H), 6.77 (d, *J* = 6.0 Hz, 1 H), 3.40-3.16 (m, 9 H), 1.70-1.37 (m, 18 H).

Step C: Synthesis of *cis*-N²-(4-amino-cyclohexylmethyl)-N²,N²-dimethyl-quinazoline-2,4-diamine.

A solution of *cis*-{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexyl}-carbamic acid *tert*-butyl ester (1.2 g, 3 mmol) in 50% TFA in CH₂Cl₂ (20 mL) was stirred at ambient temperature. After 30 minutes, the mixture was concentrated and the residue was diluted with 1 M aqueous sodium hydroxide. The aqueous layer was extracted with CH₂Cl₂ (twice). The combined organic layer was dried over Na₂SO₄, filtered and concentrated to give *cis*-N²-(4-amino-cyclohexylmethyl)-N²,N²-dimethyl-quinazoline-2,4-diamine (0.88 g, 98%) as a white solid.

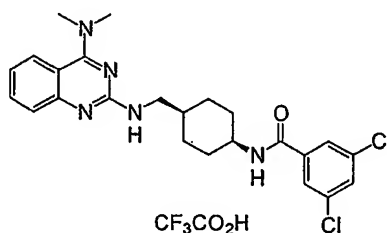
ESI MS m/e 300 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 7.85 (d, $J = 7.6$ Hz, 1 H), 7.47 (t, $J = 6.8$ Hz, 1 H), 7.27 (brs, 1 H), 7.0 (t, $J = 7.2$ Hz, 1 H), 6.66 (brs, 1 H), 3.33-3.14 (m, 9 H), 1.69-1.48 (m, 9 H).

Step D: Synthesis of *cis*- N^2 -[4-(2-ethoxy-benzylamino)-cyclohexylmethyl]- N^4 , N^4 -dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid.

A solution of *cis*- N^2 -(4-amino-cyclohexylmethyl)- N^4 , N^4 -dimethyl-quinazoline-2,4-diamine (30 mg, 0.1 mmol) and 2-ethoxy benzaldehyde (15 mg, 0.1 mmol) in MeOH (1 mL) was stirred at ambient temperature. After 3 hr, $NaBH(OAc)_3$ (85 mg, 0.4 mmol) was added and the mixture was stirred at ambient temperature for overnight. The resulting mixture was quenched with 50% DMSO in water (2 mL) and the solution was purified by preparative HPLC. The pure fractions were combined and lyophilized to give *cis*- N^2 -[4-(2-ethoxy-benzylamino)-cyclohexylmethyl]- N^4 , N^4 -dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid (33 mg, 50%) as a white solid.

ESI MS m/e 434 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 13.03 (brs, 1 H), 8.79 (brs, 1 H), 8.49 (m, 2 H), 8.15 (d, $J = 8.4$ Hz, 1 H), 7.77 (t, $J = 7.6$ Hz, 1 H), 7.40-7.33 (m, 4 H), 7.07 (d, $J = 7.6$ Hz, 1 H), 6.99 (t, $J = 7.2$ Hz, 1 H), 4.11-4.06 (m, 4 H), 3.47-3.41 (m, 8 H), 3.15 (m, 1 H), 1.90-1.60 (m, 9 H), 1.37 (t, $J = 7.2$ Hz, 3 H).

Example 2339



***cis*-3,5-Dichloro- N -{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexyl}-benzamide trifluoro-acetic acid**

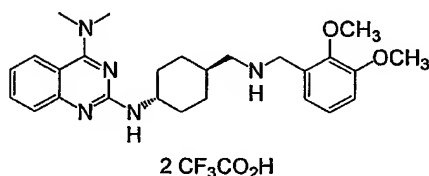
Step A: Synthesis of *cis*-3,5-dichloro- N -{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexyl}-benzamide trifluoro-acetic acid.

A solution of *cis*- N^2 -(4-amino-cyclohexylmethyl)- N^4 , N^4 -dimethyl-quinazoline-2,4-

diamine (30 mg, 0.1 mmol) and 3,5-dichlorobenzoylchloride (20.9 mg, 0.1 mmol) and pyridine (12 μ L, 0.25 mmol) in DMSO (1 mL) was stirred at ambient temperature for overnight. The mixture was purified by preparative HPLC. The pure fractions were combined and lyophilized to give *cis*-3,5-dichloro-*N*-{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexyl}-benzamide trifluoro-acetic acid. (18 mg, 31%) as a white solid.

ESI MS m/e 472 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 12.13 (brs, 1 H), 8.34 (d, $J = 7.2$ Hz, 1 H), 8.15 (d, $J = 8.8$ Hz, 1 H), 8.06 (brs, 1 H), 7.82-7.73 (m, 4 H), 7.45 (d, $J = 7.6$ Hz, 1 H), 7.36 (t, $J = 7.6$ Hz, 1 H), 3.9 (m, 1 H), 3.47-3.25 (m, 8 H), 1.83-1.56 (m, 9 H).

Example 2340



trans-*N*²-{4-[(2,3-Dimethoxy-benzylamino)-methyl]-cyclohexyl}-*N*⁴,*N*⁴-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid

Step A: Synthesis of *trans*-4-(*tert*-butoxycarbonylamino-methyl)-cyclohexanecarboxylic acid.

To a solution of *trans*-4-amino-cyclohexanecarboxylic acid (37.7 g, 0.24 mol) in a mixture of dioxane (250 ml) and water (200 ml) cooled in an ice bath were added 1 M aqueous sodium hydroxide (10.07 g, 0.25 mol) and (Boc)₂O (57.6 g, 0.26 mol). The reaction mixture was stirred at ambient temperature. After 3 hr, the mixture was concentrated and the residue was dissolved in water. The aqueous layer was washed with Et₂O (3 times). The aqueous layer was cooled in an ice bath and acidified with 1 M aqueous HCl (pH = 2) and the resulting white precipitate was dried to give *trans*-4-(*tert*-butoxycarbonylamino-methyl)-cyclohexanecarboxylic acid (47.4 g, 76.8%) as a white solid.

ESI MS m/e 258 $M + H^+$; 1H NMR (400 MHz, CDCl₃) δ 11.95 (brs, 1 H), 6.79 (t, $J = 6.0$ Hz, 1 H), 2.76 (t, $J = 6.0$ Hz, 2 H), 2.11 (m, 1 H), 1.87 (m, 2 H), 1.69 (m, 2 H), 1.36 (s,

9 H), 1.27 (m, 3 H), 0.9 (m, 2 H).

Step B: Synthesis of *trans*-[4-(*tert*-butoxycarbonylamino-methyl)-cyclohexyl]-carbamic acid benzyl ester.

To a solution of *trans*-4-(*tert*-butoxycarbonylamino-methyl)-cyclohexanecarboxylic acid (46.9 g, 0.18 mol) in benzene (300 mL) were added triethylamine (24.2 g, 0.24 mol) and diphenylphosphoryl azide (55.9 g, 0.20 mol). The reaction mixture was stirred at 80 °C for 1 hr. To the mixture was added benzyl alcohol (25.9 g, 0.24 mol) and stirred at 100 °C for 4 hr. The mixture was subsequently cooled to ambient temperature for overnight, concentrated, and the resulting pale orange solid dissolved in EtOAc. The organic layer was washed with water (three times), concentrated, and the residue was purified by column chromatography (silica gel, 50% EtOAc in hexane) to give *trans*-[4-(*tert*-butoxycarbonylamino-methyl)-cyclohexyl]-carbamic acid benzyl ester (66.7g, 100%) as a white solid.

ESI MS m/e 363 $M + H^+$; 1H NMR (400 MHz, $CDCl_3$) δ 7.24-7.23 (m, 5 H), 5.06 (s, 2 H), 4.57 (m, 2 H), 3.44 (brs, 1 H), 2.97 (t, $J = 6.4$ Hz, 2 H), 2.04 (m, 2 H), 1.79 (m, 2 H), 1.43 (s, 9 H), 1.08-0.76 (m, 5 H).

Step C: Synthesis of *trans*-(4-amino-cyclohexylmethyl)-carbamic acid *tert*-butyl ester.

To a solution of *trans*-[4-(*tert*-butoxycarbonylamino-methyl)-cyclohexyl]-carbamic acid benzyl ester (5.32 g, 0.015 mol) in EtOH (200 mL) was added 10% Pd/C (50 mg). The mixture was stirred at ambient temperature under hydrogen atmosphere for 4 hr. The resulting mixture was filtered through a pad of celite and concentrated. The residue was purified by column chromatography (silica gel, 3% 2 M $NH_3/MeOH$ in CH_2Cl_2) to give *trans*-(4-amino-cyclohexylmethyl)-carbamic acid *tert*-butyl ester as a colorless solid (3.197 g, 95.4%).

ESI MS m/e 229 $M + H^+$; 1H NMR (400 MHz, $CDCl_3$) δ 8.44 (brs, 1 H), 4.59 (b, 1 H), 2.96 (m, 2 H), 2.08 (m, 2 H), 1.83 (m, 2 H), 1.43 (s, 9 H), 1.08 (m, 5 H).

Step D: Synthesis of *trans*- N^2 -(4-aminomethyl-cyclohexyl)- N^f, N^f -dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid

A mixture of *trans*-(4-amino-cyclohexylmethyl)-carbamic acid *tert*-butyl ester

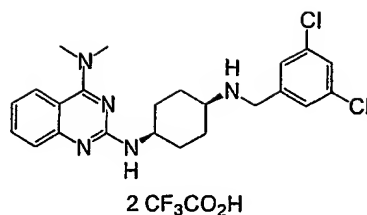
(0.24 g, 1 mmol) and (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B of example 1 (0.32 g, 1.4 mmol) in 2-propanol (5 mL) was heated to 170 °C for 30 min using a Smith Microwave Synthesizer. This procedure was repeated 19 times. The reaction mixtures were combined and purified by column chromatography (silica gel) to give 1.13 g of a yellow solid. The yellow solid was dissolved in 50% TFA in CH₂Cl₂ (20 mL) and the mixture was stirred at ambient temperature. After 10 hours, the mixture was concentrated and the residue was purified by preparative HPLC. The pure fractions were combined and lyophilized to give *trans*-*N*²-(4-aminomethyl-cyclohexyl)-*N*¹,*N*¹-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid (0.49 g, 5%) as a white solid.

ESI MS *m/e* 300 M + H⁺; ¹H NMR (400 MHz, CDCl₃) δ 9.16 (d, *J* = 5.6 Hz, 1 H), 8.11 (m, 2 H), 7.86 (d, *J* = 8.0 Hz, 1 H), 7.51 (t, *J* = 7.6 Hz, 1 H), 7.41 (d, *J* = 8.0 Hz, 1 H), 7.18 (t, *J* = 6.8 Hz, 1 H), 3.8 (brs, 1 H), 3.47 (s, 6 H), 2.10 (m, 2 H), 1.92 (m, 2 H), 1.42-1.12 (m, 5 H).

Step E: Synthesis of *trans*-*N*²-{4-[(2,3-dimethoxy-benzylamino)-methyl]-cyclohexyl}-*N*¹,*N*¹-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid.

A mixture of 2,3-dimethoxy benzaldehyde (15 mg, 0.09 mmol), *trans*-*N*²-(4-aminomethyl-cyclohexyl)-*N*¹,*N*¹-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid (28 mg, 0.053 mmol), NaBH(OAc)₃ (76 mg, 0.36 mmol), and MeOH (2 mL) was heated at 100 °C for 40 seconds using a Smith Microwave Synthesizer. The resulting mixture was purified by preparative HPLC. The pure fractions were combined and lyophilized to give *trans*-*N*²-{4-[(2,3-dimethoxy-benzylamino)-methyl]-cyclohexyl}-*N*¹,*N*¹-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid (10.2 mg, 28 %).

ESI MS *m/e* 450 M + H⁺; ¹H NMR (400 MHz, CDCl₃) δ 9.68 (d, *J* = 6.0 Hz, 1 H), 9.41 (brs, 1 H), 7.85 (d, *J* = 7.6 Hz, 1 H), 7.52 (t, *J* = 7.2 Hz, 1 H), 7.46 (d, *J* = 8.0 Hz, 1 H), 7.19 (t, *J* = 7.2 Hz, 1 H), 7.09 (t, *J* = 8.0 Hz, 1 H), 6.98 (d, *J* = 7.2 Hz, 1 H), 6.90 (d, *J* = 7.6 Hz, 1 H), 4.16 (s, 2 H), 3.96 (s, 3 H), 3.87 (s, 3 H), 3.75 (m, 1 H), 3.47 (m, 6 H), 2.80 (m, 2 H), 2.11 (m, 2 H), 1.86 (m, 2 H), 1.48-1.50 (m, 5 H).

Example 2341

***cis*-N²-[4-(3,5-Dichloro-benzylamino)-cyclohexyl]-N⁴,N⁴-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid**

Step A: Synthesis of *cis*-(4-*tert*-butoxycarbonylamino-cyclohexyl)-carbamic acid benzyl ester.

To a suspension of *cis*-4-*tert*-butoxycarbonylamino-cyclohexanecarboxylic acid (50.0 g, 206 mmol) in benzene were added triethylamine (26.9 g, 266 mmol) and phosphorazidic acid diphenyl ester (62.2 g, 226 mmol). The reaction mixture was stirred at 80°C for 1 hr. Benzyl alcohol (31.4 g, 290 mmol) was added and the mixture was stirred at reflux for 24 hr. The reaction mixture was concentrated and the residue was dissolved in EtOAc and H₂O. The organic layer was separated and the aqueous layer was extracted with EtOAc (twice). The combined organic layer was dried over MgSO₄, filtered, concentrated, and purified by flash chromatography (silica gel, 30% EtOAc in hexane) to give *cis*-(4-*tert*-butoxycarbonylamino-cyclohexyl)-carbamic acid benzyl ester (54.1 g, 76%) as a colorless oil.

ESI MS *m/e* 349 M + H⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.34-7.28 (m, 5 H), 7.12 (d, *J* = 5.6 Hz, 1 H), 6.62 (brs, 1 H), 4.98 (s, 2 H), 3.39-3.37 (m, 2 H), 1.60-1.45 (m, 8 H), 1.37 (s, 9 H).

Step B: Synthesis of *cis*-(4-amino-cyclohexyl)-carbamic acid *tert*-butyl ester.

Using the procedure for the step C of example 2340, the title compound was obtained.

ESI MS *m/e* 215 M + H⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 6.60 (d, *J* = 6.0 Hz, 1 H), 3.30-3.28 (m, 1 H), 2.74 (s, 1 H), 1.59-1.51 (m, 2 H), 1.45-1.37 (m, 15 H).

Step C: Synthesis of *cis*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-

carbamic acid *tert*-butyl ester.

A solution of *cis*-(4-amino-cyclohexyl)-carbamic acid *tert*-butyl ester (0.5 g, 2.3 mmol), (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B in example 1 (0.53, 2.6 mmol), diisopropylethylamine (1.22 mL, 7.0 mmol) and 2-propanol (1.0 mL) was heated using a Smith Microwave Synthesizer at 170 °C for 1 hour. This reaction procedure was repeated 39 more times and the resulting reaction mixtures were combined. The mixture was concentrated and the residue was purified by column chromatography (silica gel, 2% to 4% 2 M NH₃/MeOH in CH₂Cl₂) to give *cis*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-carbamic acid *tert*-butyl ester (22.1 g, 0.057 mol, 61%) as a colorless oil.

ESI MS *m/e* 386 M + H⁺; ¹H NMR (400 MHz, DMSO-d₆) δ 7.85 (d, *J* = 8.0 Hz, 1 H), 7.47 (t, *J* = 8.4 Hz, 1 H), 7.27 (d, *J* = 8.0 Hz, 1 H), 7.00 (t, *J* = 7.6 Hz, 1 H), 6.60 (brs, 1 H), 6.18 (brs, 1 H), 3.89-3.88 (m, 1 H), 3.39 (brs, 1 H), 3.19 (s, 6 H), 1.77-1.71 (m, 2 H), 1.68-1.52 (m, 6 H), 1.38 (s, 9 H).

Step D: Synthesis of *cis*-N²-(4-amino-cyclohexyl)-N⁴,N⁴-dimethyl-quinazolin-2,4-diamine.

Using the procedure for the step C of example 2338, the title compound was obtained.

ESI MS *m/e* 286 M + H⁺; ¹H NMR (400 MHz, DMSO-d₆) δ 7.84 (d, *J* = 8.4 Hz, 1 H), 7.45 (t, *J* = 6.8 Hz, 1 H), 7.26 (d, *J* = 8.4 Hz, 1 H), 6.99 (t, *J* = 7.6 Hz, 1 H), 6.20 (brs, 1 H), 3.90-3.89 (m, 1 H), 3.18 (s, 6 H), 2.79 (s, 1 H), 1.74-1.71 (m, 2 H), 1.57-1.41 (m, 8 H).

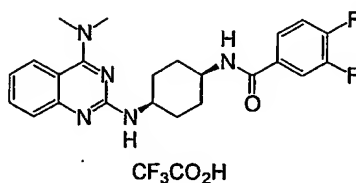
Step E: Synthesis of *cis*-N²-[4-(3,5-dichloro-benzylamino)-cyclohexyl]-N⁴,N⁴-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid.

To a solution of *cis*-N²-(4-amino-cyclohexyl)-N⁴,N⁴-dimethyl-quinazolin-2,4-diamine (31.4 mg, 0.11 mmol) in MeOH (0.5 mL) was added 3,5-dichlorobenzaldehyde (17.5 mg, 0.10 mmol). The mixture was stirred at ambient temperature for 0.5 hr and sodium triacetoxyborohydride (85 mg, 0.40 mmol) was added. The mixture was stirred for overnight and the reaction was quenched with 50% DMSO in water (1.0 mL). The mixture was purified by preparative HPLC. The pure fractions were combined and lyophilized to give *cis*-N²-[4-(3,5-dichloro-benzylamino)-cyclohexyl]-N⁴,N⁴-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid (23 mg, 0.041 mmol, 37%) as a white

solid.

ESI MS m/e 444 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 13.55 (s, 1 H), 8.90 (brs, 3 H), 8.17 (d, $J = 8.0$ Hz, 1 H), 7.79 (t, 7.6 Hz, 1 H), 7.68 (s, 1 H), 7.61 (s, 2 H), 7.41 (d, $J = 7.6$ Hz, 1 H), 7.36 (t, $J = 7.6$ Hz, 1 H), 4.23 (s, 2 H), 4.07 (s, 1 H), 3.48 (s, 6 H), 2.00-1.92 (m, 4 H), 1.82-1.74 (m, 4 H).

Example 2342

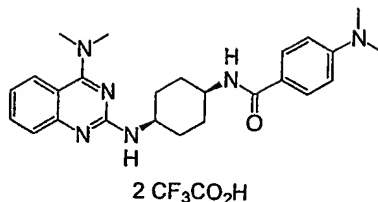


cis-N-[4-(4-Dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-3,4-difluorobenzamide trifluoro-acetic acid.

Step A: Synthesis of *cis-N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-3,4-difluorobenzamide trifluoro-acetic acid.

Using the procedure for the step A of example 2333, the title compound was obtained.

ESI MS m/e 426 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 12.46 (brs, 1 H), 8.36 (s, 1 H), 8.15 (d, $J = 8.0$ Hz, 1 H), 7.97 (brs, 1 H), 7.94-7.89 (m, 1 H), 7.77-7.73 (m, 2 H), 7.56-7.49 (m, 1 H), 7.41 (brs, 1 H), 7.36 (t, $J = 7.6$ Hz, 1 H), 4.07 (m, 1 H), 3.87 (m, 1 H), 3.47 (brs, 6 H), 1.89 (m, 2 H), 1.74 (m, 6 H).

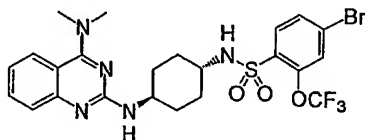
Example 2343

***cis*-4-Dimethylamino-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-benzamide ditrifluoro-acetic acid**

Step A: Synthesis of *cis*-4-dimethylamino-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-benzamide ditrifluoro-acetic acid.

To a solution of 4-dimethylaminobenzoic acid (16.5 mg, 0.10 mmol) in DMF (0.5 mL) were added HATU (45.6 mg, 0.12 mmol), diisopropylethylamine (34.8 μ L, 0.20 mmol), and *cis*-*N*²-(4-amino-cyclohexyl)-*N*⁴,*N*⁴-dimethyl-quinazolin-2,4-diamine obtained in step D of example 2341 (28.5 mg, 0.10 mmol) and stirred at ambient temperature for overnight. The resulting mixture was diluted with DMSO (0.5 mL) and purified by preparative HPLC. The pure fractions combined and lyophilized to give *cis*-4-dimethylamino-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-benzamide ditrifluoro-acetic acid (34.1 mg, 0.052mmol, 52%) as a white solid.

ESI MS *m/e* 433 *M* + *H*⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.73 (s, 1 H), 8.34 (s, 1 H), 8.16 (d, *J* = 8.0 Hz, 1 H), 7.78-7.70 (m, 4 H), 7.43 (d, *J* = 7.6 Hz, 1 H), 7.35 (t, *J* = 8.0 Hz, 1 H), 6.67 (d, *J* = 8.8 Hz, 2 H), 4.05 (m, 1 H), 3.86 (m, 1 H), 3.47 (s, 6 H), 2.95 (s, 3 H), 2.53 (s, 3 H), 1.91 (m, 2 H), 1.75-1.72 (m, 6 H).

Example 2344

***trans*-4-Bromo-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-2-trifluoromethoxy-benzenesulfonamide**

Step A: Synthesis of *trans*-(4-amino-cyclohexyl)-carbamic acid *tert*-butyl ester.

To a solution of *trans*-1,4-diamino-cyclohexane (10 g, 0.088 mol) in 1,4-dioxane (400 mL) was added a solution of (Boc)₂O (4.78 g, 0.022 mol) in 1,4-dioxane (100 mL) over 30 min. The mixture was stirred at ambient temperature for overnight and then the dioxane was removed in vacuo. The resulting precipitate was dissolved in H₂O (500 mL) and left to sit for 1 hour. During this time, the di-Boc-protected diamino-cyclohexane fell out as a white crystalline precipitate. This was subsequently filtered from the aqueous solvent. The aqueous layer was extracted with EtOAc (three times). The organic layers were combined and washed with H₂O. The organic layer was dried over MgSO₄ and concentrated to give *trans*-(4-amino-cyclohexyl)-carbamic acid *tert*-butyl ester (4 g, 0.019 mol, 85%).

ESI MS *m/e* 215 M + H⁺; ¹H NMR (400 MHz, DMSO-d₆) δ 6.63 (d, *J* = 8.0 Hz, 1 H), 3.11-3.09 (m, 1 H), 2.44-2.37 (m, 1 H), 1.70-1.67 (m, 4 H), 1.41-1.31 (m, 11 H), 1.20-0.95 (m, 4 H).

Step B: Synthesis of *trans*-[4-(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-cyclohexyl]-carbamic acid *tert*-butyl ester.

To a solution of *trans*-(4-amino-cyclohexyl)-carbamic acid *tert*-butyl ester (1 g, 0.0047 mol) in CH₂Cl₂ were added diisopropylethylamine (1.63 mL, 0.0093 mol) and 4-bromo-2-trifluoromethoxy-benzenesulfonyl chloride (1.03 mL, 0.0051 mol). The reaction mixture was stirred at ambient temperature for 1 hr and then washed with water. The aqueous layer was extracted with CH₂Cl₂ (twice), the organic layers were combined, dried over MgSO₄, and concentrated. The resulting precipitate was recrystallized with CH₂Cl₂ and hexanes to give *trans*-[4-(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-cyclohexyl]-carbamic acid *tert*-butyl ester (2.39 g, 0.0046 mol, 99%).

ESI MS *m/e* 517 M + H⁺; ¹H NMR (400 MHz, DMSO-d₆) δ 7.99 (d, *J* = 7.6 Hz, 1 H), 7.85 (d, *J* = 8.0 Hz, 1 H), 7.79-7.77 (m, 1 H), 6.67 (d, *J* = 8.0 Hz, 1 H), 3.14-2.94 (m, 2 H), 1.70-1.60 (m, 4 H), 1.34 (s, 9 H), 1.30-1.18 (m, 2 H), 1.14-1.03 (m, 2 H).

Step C: Synthesis of *trans*-N-(4-amino-cyclohexyl)-4-bromo-2-trifluoromethoxy-benzenesulfonamide.

Using the procedure for the step C of example 2338, the title compound was obtained.

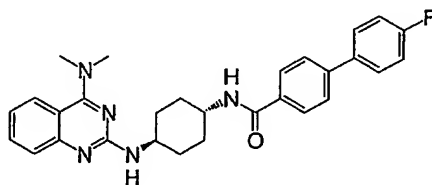
ESI MS m/e 417/419 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 7.85 (d, $J = 8.4$ Hz, 1 H), 7.79-7.76 (m, 3 H), 3.32 (brs, 2 H), 3.03-2.95 (m, 1 H), 2.41-2.36 (m, 1 H), 1.67-1.57 (m, 4 H), 1.28-1.18 (m, 2 H), 0.99-0.89 (m, 2 H).

Step D: Synthesis of *trans*-4-bromo-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-2-trifluoromethoxy-benzenesulfonamide.

To a solution of *trans*-*N*-(4-amino-cyclohexyl)-4-bromo-2-trifluoromethoxy-benzenesulfonamide (100 mg, 0.24 mmol) in 2-propanol (0.5 mL) was added (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B of example 1 (54.7 mg, 0.26 mmol). The mixture was heated using a Smith Microwave Synthesizer at 170 °C for 15 min. The mixture was concentrated and the residue was purified by chromatography (2% to 4% 2 M $NH_3/MeOH$ in CH_2Cl_2) to give *trans*-4-bromo-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-2-trifluoromethoxy-benzenesulfonamide (42 mg, 0.71 mmol, 30%) as a white solid.

ESI MS m/e 588/590 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 8.02 (d, $J = 7.6$ Hz, 1 H), 7.88 (d, $J = 8.4$ Hz, 1 H), 7.82-7.77 (m, 3 H), 7.45-7.41 (m, 1 H), 7.25-7.41 (m, 1 H), 6.99 (t, $J = 7.2$ Hz, 1 H), 6.37 (brs, 1 H), 3.68-3.67 (m, 1 H), 3.16 (s, 6 H), 3.09-3.02 (m, 1 H), 1.89-1.86 (m, 2 H), 1.69-1.67 (m, 2 H), 1.40-1.17 (m, 4 H).

Example 2345



***trans*-4'-Fluoro-biphenyl-4-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-amide.**

Step A: Synthesis of 4'-fluoro-biphenyl-4-carboxylic acid.

To a solution of 4-bromobenzoic acid (5 g, 0.025 mol) in THF (150 mL) under an

atmosphere of argon were added tetrakis(triphenylphosphine) palladium(0) (862 mg, 0.75 mmol), 2 M aqueous Na_2CO_3 (30 mL), and a solution 4-fluorophenylboronic acid (3.48 g, 0.025 mol) in a minimal amount of ethanol (~10 mL). The resulting reaction mixture was stirred at reflux under an argon atmosphere for overnight. The reaction mixture was cooled to ambient temperature and acidified with addition of 1 M HCl aqueous. The aqueous layer was extracted with Et_2O (three times). The organic layers were combined, dried over MgSO_4 , filtered and concentrated. The resulting precipitate was crystallized in Et_2O and hexane to give 4'-fluoro-biphenyl-4-carboxylic acid (4.4 g, 0.020 mol, 82%) as a white solid.

^1H NMR (400 MHz, DMSO-d_6) δ 12.96 (s, 1 H), 8.00-7.98 (m, 2 H), 7.78-7.75 (m, 4 H), 7.34-7.31 (m, 2 H).

Step B: Synthesis of *trans*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-carbamic acid *tert*-butyl ester.

Using the procedure for the step D of example 2344, the title compound was obtained.

ESI MS m/e 386 $\text{M} + \text{H}^+$; ^1H NMR (400 MHz, DMSO-d_6) δ 7.83 (d, $J = 8.0$ Hz, 1 H), 7.46 (t, $J = 6.8$ Hz, 1 H), 7.27-7.25 (m, 1 H), 6.99 (t, $J = 7.2$ Hz, 1 H), 6.71 (d, $J = 8.4$ Hz, 1 H), 6.38 (brs, 1 H), 3.72 (m, 1 H), 3.17 (s, 6 H), 1.92-1.90 (m, 2 H), 1.79-1.76 (m, 2 H), 1.37 (s, 9 H), 1.34-1.23 (m, 4 H).

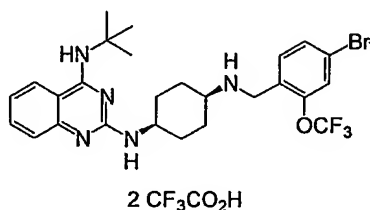
Step C: Synthesis of *trans*-4'-fluoro-biphenyl-4-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-amide.

To a solution of *trans*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-carbamic acid *tert*-butyl ester (0.76 g, 0.20 mmol) in CH_2Cl_2 (20 mL) was added TFA (304 μL , 0.39 mmol). The solution was stirred at ambient temperature for 4 hr. The resulting mixture was concentrated and the residue was dissolved in CH_2Cl_2 . The organic layer was washed with a dilute aqueous NaOH and aqueous NaHCO_3 solution. The aqueous layer was extracted with CH_2Cl_2 (twice) and the organic layers combined, dried over MgSO_4 , and concentrated. To a solution of the residue (0.1 g) and 4'-fluoro-biphenyl-4-carboxylic acid (76 mg, 0.35 mmol) in CH_2Cl_2 were added HOAt (62 mg, 0.46 mmol), WSC•HCl (87 mg, 0.46 mmol), and diisopropylethylamine (31 μL , 0.18 mmol). The mixture was stirred for 1 hr at ambient temperature and the reaction was quenched with

water. The aqueous layer was extracted with CH_2Cl_2 (twice). The organic layers were combined, dried over MgSO_4 , concentrated and the residue purified by column chromatography (silica gel, 2% to 4% 2 M NH_3/MeOH in CH_2Cl_2) to give *trans*-4'-fluoro-biphenyl-4-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-amide (35 mg, 0.072, 21%) as a white solid.

ESI MS m/e 484 $M + H^+$; ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 8.30 (brs, 1 H), 8.12 (brs, 2 H), 7.92 (d, $J = 8.4$ Hz, 2 H), 7.77-7.72 (m, 5 H), 7.44 (brs, 1 H), 7.34-7.28 (m, 3 H), 3.82 (brs, 2 H), 3.47 (brs, 6 H), 2.04 (m, 2 H), 1.94 (m, 2 H), 1.54-1.48 (m, 4 H).

Example 2346



cis- N^2 -[4-(4-Bromo-2-trifluoromethoxy-benzylamino)-cyclohexyl]- N^4 -*tert*-butyl-quinazoline-2,4-diamine ditrifluoro-acetic acid

Step A: Synthesis of *tert*-butyl-(2-chloro-quinazolin-4-yl)-amine.

To a solution of 2,4-dichloro-quinazoline obtained in step B of example 1 (4 g, 20 mmol) in THF (50 mL) were added *tert*-butyl amine (2.15 mL, 20.5 mmol) and diisopropylethylamine (3.5 mL, 21 mmol). The mixture was stirred at ambient temperature for 2 hr. The mixture was concentrated and the residue was dissolved in EtOAc. The organic layer was washed with water, dried over Na_2SO_4 , and filtered. The mixture was concentrated to give *tert*-butyl-(2-chloro-quinazolin-4-yl)-amine as a white solid (3 g, 64%).

ESI MS m/e 236 $M + H^+$; ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 8.40 (d, $J = 8.4$ Hz, 1 H), 7.75-7.36 (m, 2 H), 7.58 (d, $J = 8.4$ Hz, 1 H), 7.48 (t, $J = 7.2$ Hz, 1 H), 1.52 (s, 9 H).

Step B: Synthesis of *cis*- N^2 -(4-amino-cyclohexyl)- N^4 -*tert*-butyl-quinazoline-2,4-diamine.

To a suspension of *cis*-(4-amino-cyclohexyl)-carbamic acid *tert*-butyl ester (122

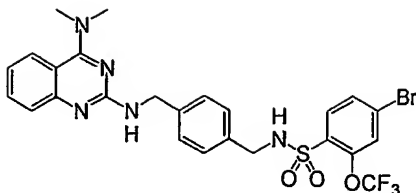
mg, 0.57 mmol) in 2-propanol (2 mL) were added *tert*-butyl-(2-chloro-quinazolin-4-yl)-amine (100 mg, 0.42 mmol) and diisopropylethylamine (180 μ L, 1 mmol) and the mixture was heated at 170 °C for 1 hr using a Smith Microwave Synthesizer. The resulting solution was concentrated and purified by column chromatography (silica gel, 3% MeOH in CH₂Cl₂) to give [4-(4-*tert*-butylamino-quinazolin-2-ylamino)-cyclohexyl]-carbamic acid *tert*-butyl ester (112 mg, 65%) as a yellow solid. To a suspension of *cis*-[4-(4-*tert*-butylamino-quinazolin-2-ylamino)-cyclohexyl]-carbamic acid *tert*-butyl ester (95 mg, 0.23 mmol) in CH₂Cl₂ (3 mL) was added trifluoroacetic acid (2 mL) dropwise. The reaction mixture was stirred at ambient temperature for 2 hr. The solution was concentrated, alkalized with saturated aqueous NaHCO₃ and 1 M aqueous sodium hydroxide (pH = 9), and the aqueous layer was extracted with CH₂Cl₂ (three times). The combined organic layer was dried over MgSO₄, filtered, and concentrated. The solid was collected by filtration to give *cis*-N²-(4-amino-cyclohexyl)-N⁴-*tert*-butyl-quinazoline-2,4-diamine (44.6 mg, 53%) as a yellow solid.

ESI MS *m/e* 314 M + H⁺; ¹H NMR (400 MHz, CDCl₃) δ 7.48 (t, *J* = 6.8 Hz, 1 H), 7.38 (m, 2 H), 7.04 (t, *J* = 8.0 Hz, 1 H), 5.42 (brs, 1 H), 4.15 (m, 1 H), 2.85 (m, 1 H), 1.2-1.9 (m, 17 H).

Step C: Synthesis of *cis*-N²-[4-(4-bromo-2-trifluoromethoxy-benzylamino)-cyclohexyl]-N⁴-*tert*-butyl-quinazoline-2,4-diamine ditrifluoro-acetic acid.

Using the procedure for the step C of example 2341, the title compound was obtained.

ESI MS *m/e* 566 M + H⁺; ¹H NMR (400 MHz, CDCl₃) δ 9.36 (d, *J* = 8.0 Hz, 1 H), 7.67-7.64 (m, 2 H), 7.53-7.48 (m, 3 H), 7.43 (s, 1 H), 7.33 (m, 1 H), 6.17 (s, 1 H), 4.45 (m, 1 H), 4.28 (s, 2 H), 3.35 (m, 1 H), 2.14-1.6 (m, 17 H).

Example 2347

4-Bromo-*N*-{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-benzyl}-2-trifluoromethoxy-benzenesulfonamide

Step A: Synthesis of {4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-benzyl}-carbamic acid tert-butyl ester.

Using the procedure for the step D of example 2330, the title compound was obtained.

ESI MS m/e 377 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 8.38 (brs, 1 H), 8.08 (brs, 1 H), 7.70 (brs, 1 H), 7.47 (brs, 1 H), 7.36 (t, $J = 6.2$ Hz, 1 H), 7.30 (d, $J = 8.0$ Hz, 3 H), 7.16 (d, $J = 7.6$ Hz, 2 H), 4.60 (d, $J = 6.4$ Hz, 2 H), 4.07 (d, $J = 6.0$ Hz, 2 H), 3.39 (s, 6 H), 1.37 (s, 9 H).

Step B: Synthesis of *N*²-(4-aminomethyl-benzyl)-*N*¹,*N*¹-dimethyl-quinazoline-2,4-diamine hydrochloride.

To a cooled solution of {4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-benzyl}-carbamic acid tert-butyl ester (3.90 g, 9.57 mmol) in MeOH was added 1 M HCl in Et₂O (67.0 ml, 67.0 mmol) and the solution was stirred for overnight. The resulting mixture was concentrated to give *N*²-(4-aminomethyl-benzyl)-*N*¹, *N*¹-dimethyl-quinazoline-2,4-diamine hydrochloride as a white crystalline solid (3.48 g, 95.6%).

ESI MS m/e 308.2 $M + H^+$; 1H NMR (400 MHz, CD₃OD) δ 8.16 (d, $J = 7.2$ Hz, 1 H), 7.75 (brs, 1 H), 7.48 (m, 5 H), 7.39 (brs, 1 H), 4.76 (s, 2 H), 4.12 (s, 2 H), 3.51 (m, 6 H).

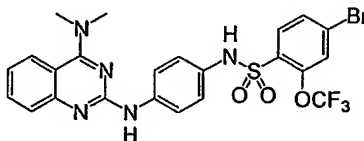
Step C: Synthesis of 4-bromo-*N*-{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-benzyl}-2-trifluoromethoxy-benzenesulfonamide.

A solution of *N*²-(4-aminomethyl-benzyl)-*N*¹,*N*¹-dimethyl-quinazoline-2,4-diamine hydrochloride (50.0 mg, 0.131 mmol), 4-bromo-2-trifluoromethoxy-benzenesulfonyl chloride (53.3 mg, 0.157 mmol) and diisopropylethylamine (91 μ l, 0.524 mmol) in 2-

propanol (1.5 mL) was stirred at ambient temperature for 2 hr. The resulting mixture was concentrated, and the residue was purified by column chromatography (silica gel, 10% MeOH in CH₂Cl₂) to give 4-bromo-*N*-{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-benzyl}-2-trifluoromethoxy-benzenesulfonamide as a white crystalline compound (40 mg, 50%).

ESI MS *m/e* 612 *M* + *H*⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.51 (t, *J* = 6.4 Hz, 1 H), 8.06 (brs, 1 H), 7.76-7.67 (m, 4 H), 7.54-7.41 (m, 2 H), 7.24 (d, *J* = 7.6 Hz, 3 H), 7.14 (d, *J* = 8.0 Hz, 2 H), 4.56 (d, *J* = 6.0 Hz, 2 H), 4.08 (d, *J* = 6.0 Hz, 2 H), 3.36 (s, 6 H).

Example 2348



4-bromo-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-phenyl]-2-trifluoromethoxy-benzenesulfonamide

Step A: Synthesis of (4-amino-phenyl)-carbamic acid *tert*-butyl ester.

Using the procedure for the step A of example 2344, the title compound was obtained.

ESI MS *m/e* 209 *M* + *H*⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.75 (s, 1 H), 7.03 (d, *J* = 7.6 Hz, 2 H), 6.43 (dt, *J* = 9.5, 2.7 Hz, 2 H), 4.71 (s, 2 H), 1.43 (s, 9 H).

Step B: Synthesis of *N*²-(4-amino-phenyl)-*N*⁴,*N*⁴-dimethyl-quinazoline-2,4-diamine hydrochloride.

A mixture of (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B of example 1 (0.5 g, 2.6 mmol) and (4-amino-phenyl)-carbamic acid *tert*-butyl ester (0.5 g, 2.6 mmol) in CH₂Cl₂ (2 mL) was heated by Smith Synthesizer at 130 °C for 20 min. The mixture was concentrated to give [4-(4-dimethylamino-quinazolin-2-ylamino)-phenyl]-carbamic acid *tert*-butyl ester as a pale yellow solid (0.86 g, 87%). The reaction was repeated six times, and the total product combined was 8.5 g. To a solution of above product (8.5 g, 22.4 mmol) in MeOH (250 mL) was added 4 M HCl in dioxane (8.4 mL,

33.6 mmol) dropwise, and the mixture was stirred at ambient temperature for overnight. The mixture was concentrated to give *N*²-(4-amino-phenyl)-*N*¹,*N*¹-dimethyl-quinazoline-2,4-diamine hydrochloride as a pale pink solid (6.2 g, 87.5%).

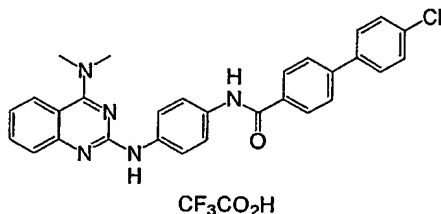
ESI MS *m/e* 280 *M* + *H*⁺; ¹H NMR (400 MHz, D₂O) δ 7.84 (d, *J* = 8.8 Hz, 1 H), 7.54 (td, *J* = 7.8, 1.2 Hz, 1 H), 7.46 (dt, *J* = 9.5, 2.7 Hz, 2 H), 7.27-7.16 (m, 4 H), 3.35 (b, 3 H), 3.12 (b, 3 H).

Step C: Synthesis of 4-bromo-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-phenyl]-2-trifluoromethoxy-benzenesulfonamide.

Using the procedure for the step C of example 2347, the title compound was obtained.

ESI MS *m/e* 584 *M* + *H*⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 10.27 (brs, 1 H), 9.14 (brs, 1 H), 7.98 (d, *J* = 8.4 Hz, 1 H), 7.80-7.71 (m, 5 H), 7.60-7.56 (m, 1 H), 7.44 (d, *J* = 8.4 Hz, 1 H), 7.15 (t, *J* = 7.4 Hz, 1 H), 6.95 (d, *J* = 16.8 Hz, 2 H), 9.29 (s, 6 H).

Example 2349



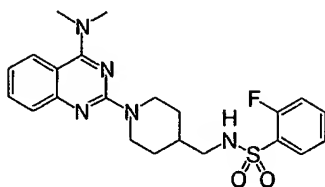
4'-Chloro-biphenyl-4-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-phenyl]-amide trifluoro-acetic acid

Synthesis of 4'-chloro-biphenyl-4-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-phenyl]-amide trifluoro-acetic acid.

A solution of *N*²-(4-amino-phenyl)-*N*¹,*N*¹-dimethyl-quinazoline-2,4-diamine hydrochloride obtained in step B of example 2348 (81.6 mg, 0.258 mmol), 4'-chloro-biphenyl-4-carboxylic acid (50.0 mg, 0.215 mmol), HATU (106 mg, 0.280 mmol), and diisopropylethylamine (150 μL, 0.860 mmol), in CH₂Cl₂ (2 mL) was stirred at ambient temperature for overnight, and the mixture was concentrated. The residue was purified by HPLC to give 4'-chloro-biphenyl-4-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-phenyl]-amide trifluoro-acetic acid as a white solid (10 mg, 9 %).

ESI MS m/e 494 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 10.33 (s, 1 H), 8.17 (d, J = 8.0 Hz, 1 H), 8.80 (d, J = 8.8 Hz, 2 H), 7.85-7.75 (m, 7 H), 7.63-7.53 (m, 6 H), 7.36 (t, J = 7.6 Hz, 1 H), 3.46 (s, 6 H).

Example 2350



N-[1-(4-Dimethylamino-quinazolin-2-yl)-piperidin-4-ylmethyl]-2-fluoro-benzenesulfonamide

Step A: Synthesis of *N*-[1-(4-dimethylamino-quinazolin-2-yl)-piperidin-4-ylmethyl]-2-fluoro-benzenesulfonamide.

To a solution of 4-aminomethyl-piperidine-1-carboxylic acid *tert*-butyl ester (60 mg, 0.28 mmol) and diisopropylethylamine (49 mL, 0.28 mmol) in CH_2Cl_2 (2 mL) was added 2-fluorobenzenesulfonyl chloride (54 mg, 0.28 mmol) and the mixture was stirred at ambient temperature for 18 hr. To the resulting mixture was added trifluoroacetic acid (0.70 mL) and stirred at ambient temperature for 18 hr. The reaction mixture was concentrated and neutralized with saturated aqueous $NaHCO_3$. The aqueous layer was extracted with EtOAc, and the organic layer was concentrated to give 2-fluoro-*N*-piperidin-4-ylmethyl-benzenesulfonamide as a pale yellow solid. To a solution of above solid (0.076 g, 0.28 mmol) and diisopropylethylamine (0.072 mL, 0.42 mmol) in 2-propanol (3 mL) was added (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B of example 1 (0.044 g, 0.21 mmol) and the resulting mixture was stirred at 100 °C for 18 hr. The mixture was concentrated, and the residue was purified by column chromatography (silica gel, 5% MeOH in CH_2Cl_2) to give *N*-[1-(4-dimethylamino-quinazolin-2-yl)-piperidin-4-ylmethyl]-2-fluoro-benzenesulfonamide as a pale yellow solid (0.024 g, 26%).

ESI MS m/e 444 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 7.98 (m, 1 H), 7.86 (m, 1 H), 7.77 (m, 1 H), 7.67 (m, 1 H), 7.47-7.29 (m, 4 H), 7.02 (m, 1 H), 4.69 (m, 2 H), 3.21 (s, 6 H), 2.76 (m, 4 H), 1.66 (m, 3 H), 1.00 (m, 2 H).

Using the procedure for example 2329 and purification by preparative HPLC, the compounds of example 2351 - 2819 were obtained.

Using the procedure for example 2331 and purification by preparative HPLC, the compounds of example 2820 - 2842 were obtained.

Using the procedure for example 2332, the compounds of example 2843 - 3003 were obtained.

Using the procedure for example 2333, the compounds of example 3004 - 3090 were obtained.

Using the procedure for example 2334, the compounds of example 3091 - 3161 were obtained.

Using the procedure for example 2335 and purification by preparative HPLC, the compounds of example 3162 - 3178 were obtained.

Using the procedure for example 2336, the compounds of example 3179 - 3208 were obtained.

Using the procedure for example 2337, the compounds of example 3209 was obtained.

Using the procedure for example 2338, the compounds of example 3210 - 3225 were obtained.

Using the procedure for example 2339, the compounds of example 3226 - 3228 were obtained.

Using the procedure for example 2340, the compounds of example 3229 - 3231 were obtained.

Using the procedure for example 2341, the compounds of example 3232 - 3393 were obtained.

Using the procedure for example 2342, the compounds of example 3394 - 3472 were obtained.

Using the procedure for example 2343, the compounds of example 3473 - 3527 were obtained.

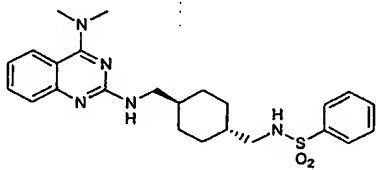
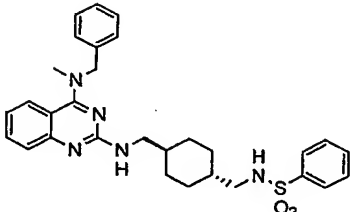
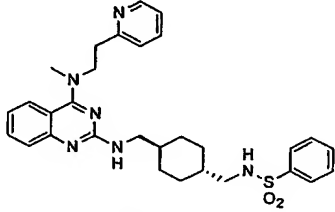
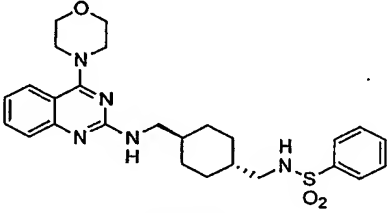
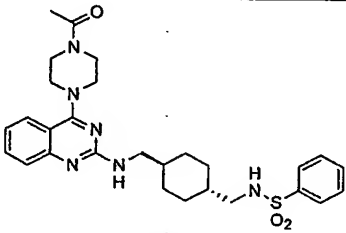
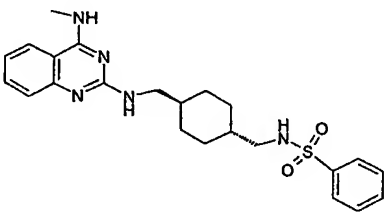
Using the procedure for example 2346, the compounds of example 3528 - 3535 were obtained.

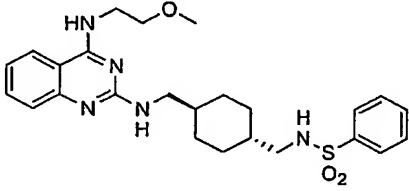
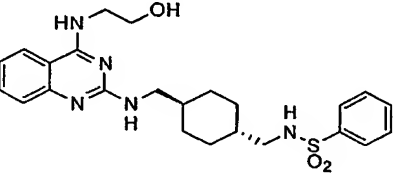
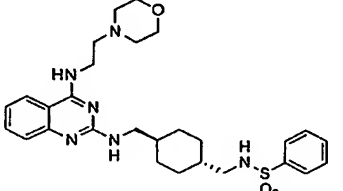
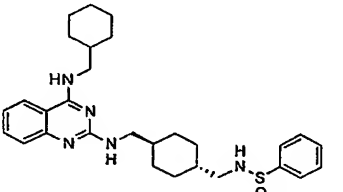
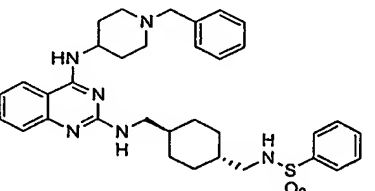
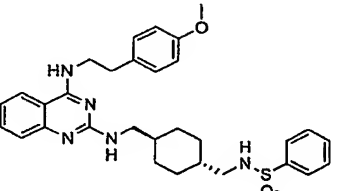
Using the procedure for example 2347 and purification by preparative HPLC, the compounds of example 3536 - 3545 were obtained.

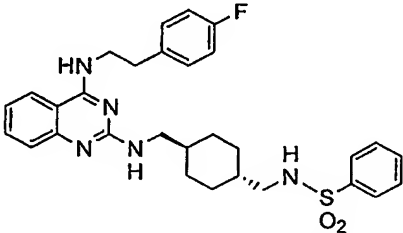
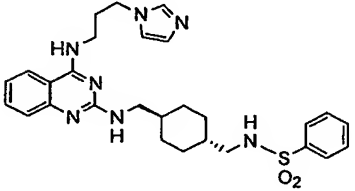
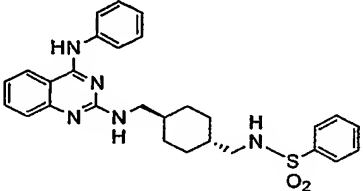
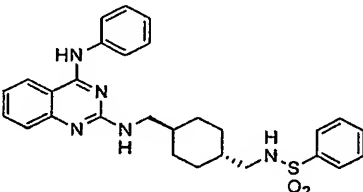
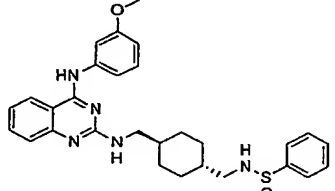
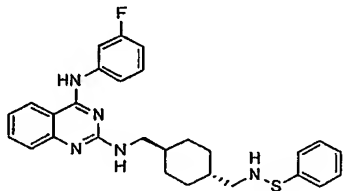
Using the procedure for example 2348 and purification by preparative HPLC, the compounds of example 3546 - 3548 were obtained.

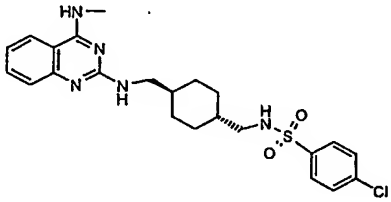
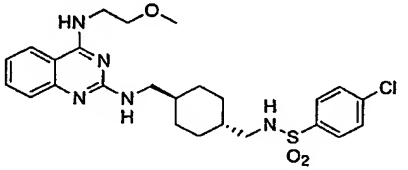
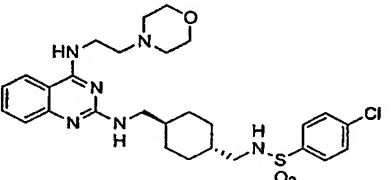
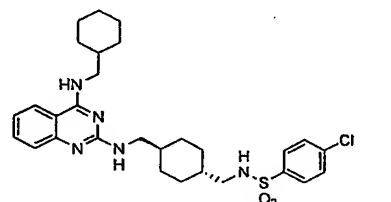
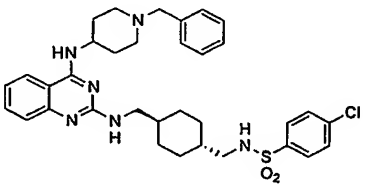
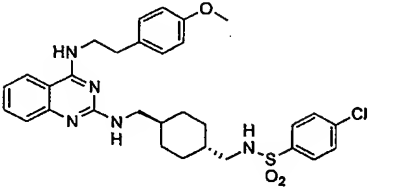
Using the procedure for example 2349, the compounds of example 3549 - 3567 were obtained.

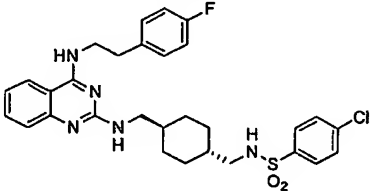
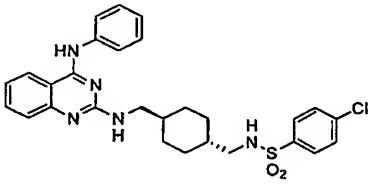
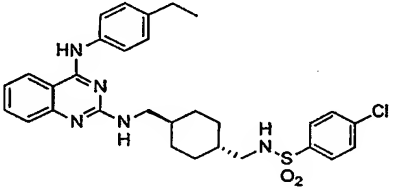
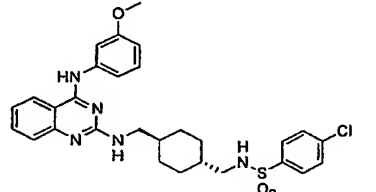
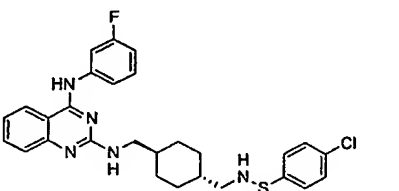
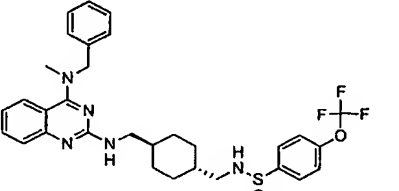
Using the procedure for example 2350 and purification by preparative HPLC, the compounds of example 3568 - 3579 were obtained.

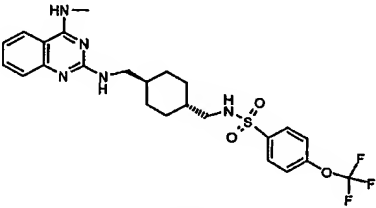
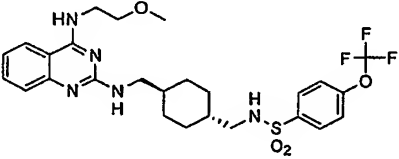
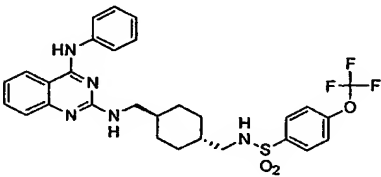
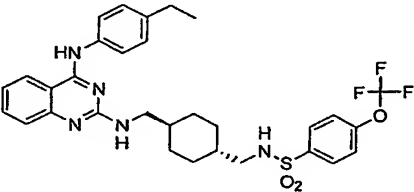
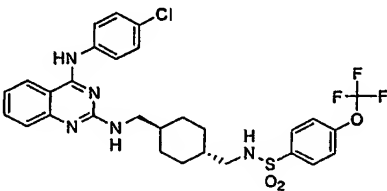
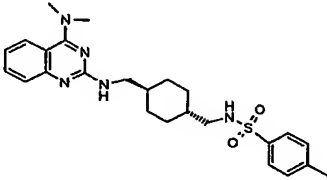
Example No.	Structure	ESI-MS	Retention Time (min)
2351	 $\text{CF}_3\text{CO}_2\text{H}$	454.0 (M + H)	3.60
2352	 $\text{CF}_3\text{CO}_2\text{H}$	530.2 (M + H)	4.02
2353	 $2\text{CF}_3\text{CO}_2\text{H}$	545.4 (M + H)	3.05
2354	 $\text{CF}_3\text{CO}_2\text{H}$	496.4 (M + H)	3.49
2355	 $\text{CF}_3\text{CO}_2\text{H}$	537.4 (M + H)	3.24
2356	 $\text{CF}_3\text{CO}_2\text{H}$	440.0 (M + H)	3.47

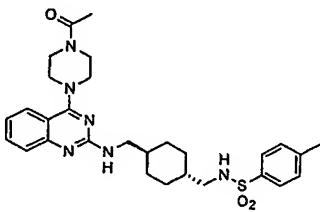
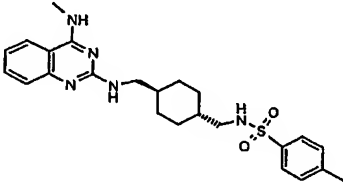
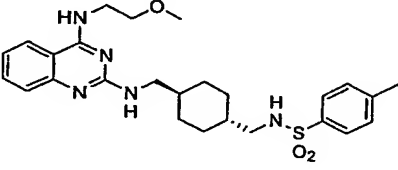
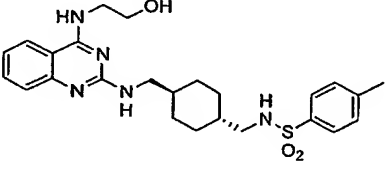
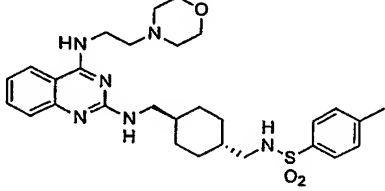
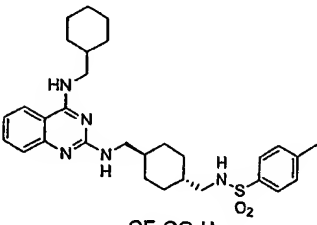
Example No.	Structure	ESI-MS	Retention Time (min)
2357	 $\text{CF}_3\text{CO}_2\text{H}$	484.4 (M + H)	3.49
2358	 $\text{CF}_3\text{CO}_2\text{H}$	470.2 (M + H)	3.20
2359	 $2\text{CF}_3\text{CO}_2\text{H}$	539.4 (M + H)	3.12
2360	 $\text{CF}_3\text{CO}_2\text{H}$	522.2 (M + H)	4.22
2361	 $2\text{CF}_3\text{CO}_2\text{H}$	599.0 (M + H)	3.48
2362	 $\text{CF}_3\text{CO}_2\text{H}$	560.2 (M + H)	3.99

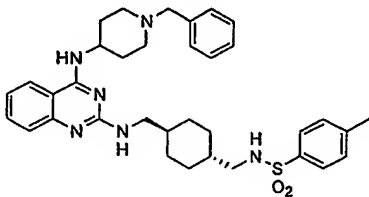
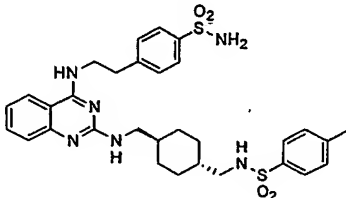
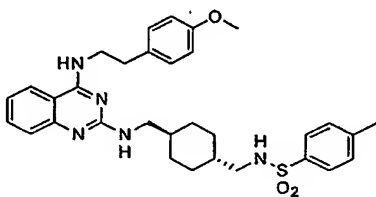
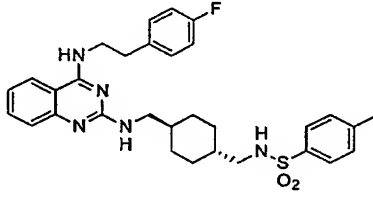
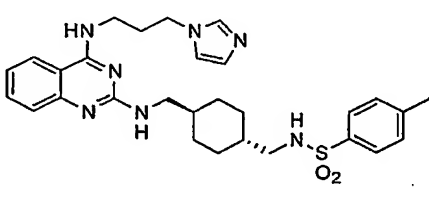
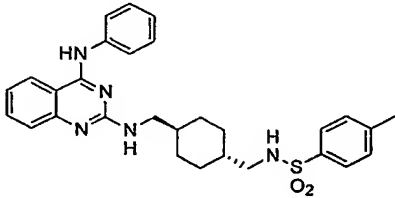
Example No.	Structure	ESI-MS	Retention Time (min)
2363	 <chem>NS(=O)(=O)c1ccc(cc1)N[C@H]2CCCC[C@H]2CN3C=NC4=CC=CC=C4N=C3N5C=CC=C5N4</chem>	548.4 (M + H)	4.06
2364	 <chem>NS(=O)(=O)c1ccc(cc1)N[C@H]2CCCC[C@H]2CN3C=NC4=CC=CC=C4N=C3N5C=CC=C5N4</chem> <chem>2CF3CO2H</chem>	534.0 (M + H)	3.11
2365	 <chem>NS(=O)(=O)c1ccc(cc1)N[C@H]2CCCC[C@H]2CN3C=NC4=CC=CC=C4N=C3N5C=CC=C5N4</chem> <chem>CF3CO2H</chem>	502.4 (M + H)	3.81
2366	 <chem>NS(=O)(=O)c1ccc(cc1)N[C@H]2CCCC[C@H]2CN3C=NC4=CC=CC=C4N=C3N5C=CC=C5N4</chem> <chem>CF3CO2H</chem>	530.2 (M + H)	4.04
2367	 <chem>NS(=O)(=O)c1ccc(cc1)N[C@H]2CCCC[C@H]2CN3C=NC4=CC=CC=C4N=C3N5C=CC=C5N4</chem> <chem>CF3CO2H</chem>	532.4 (M + H)	3.85
2368	 <chem>NS(=O)(=O)c1ccc(cc1)N[C@H]2CCCC[C@H]2CN3C=NC4=CC=CC=C4N=C3N5C=CC=C5N4</chem> <chem>CF3CO2H</chem>	520.2 (M + H)	3.86

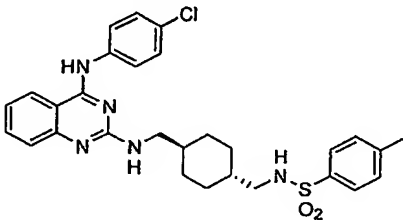
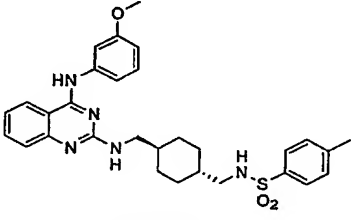
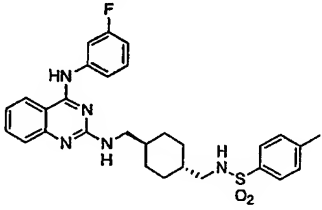
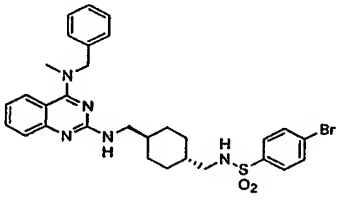
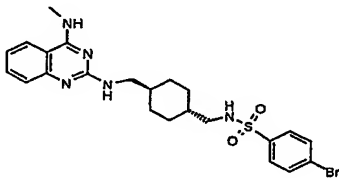
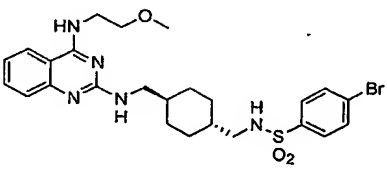
Example No.	Structure	ESI-MS	Retention Time (min)
2369	 <chem>CC1(CCN2C=NC3=CC=CC=C3N=C2N1)CC[C@H](C1=CC=C(C=C1)S(=O)(=O)N)C2=CC=CC=C2</chem> $\text{CF}_3\text{CO}_2\text{H}$	474.2 (M + H)	3.72
2370	 <chem>COCCN1C=NC2=CC=CC=C2N=C1N</chem> <chem>CC1(CCN2C=NC3=CC=CC=C3N=C2N1)CC[C@H](C1=CC=C(C=C1)S(=O)(=O)N)C2=CC=CC=C2</chem> $\text{CF}_3\text{CO}_2\text{H}$	518.2 (M + H)	3.71
2371	 <chem>C1CCN(C1)CCN2C=NC3=CC=CC=C3N=C2N</chem> <chem>CC1(CCN2C=NC3=CC=CC=C3N=C2N1)CC[C@H](C1=CC=C(C=C1)S(=O)(=O)N)C2=CC=CC=C2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	573.2 (M + H)	3.15
2372	 <chem>C1CCCCC1CN2C=NC3=CC=CC=C3N=C2N</chem> <chem>CC1(CCN2C=NC3=CC=CC=C3N=C2N1)CC[C@H](C1=CC=C(C=C1)S(=O)(=O)N)C2=CC=CC=C2</chem> $\text{CF}_3\text{CO}_2\text{H}$	556.2 (M + H)	4.38
2373	 <chem>c1ccccc1CCN2C=NC3=CC=CC=C3N=C2N</chem> <chem>CC1(CCN2C=NC3=CC=CC=C3N=C2N1)CC[C@H](C1=CC=C(C=C1)S(=O)(=O)N)C2=CC=CC=C2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	633.4 (M + H)	3.48
2374	 <chem>COc1ccc(cc1)CCN2C=NC3=CC=CC=C3N=C2N</chem> <chem>CC1(CCN2C=NC3=CC=CC=C3N=C2N1)CC[C@H](C1=CC=C(C=C1)S(=O)(=O)N)C2=CC=CC=C2</chem> $\text{CF}_3\text{CO}_2\text{H}$	594.2 (M + H)	4.23

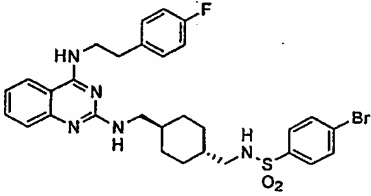
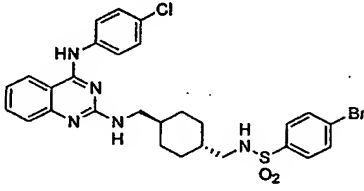
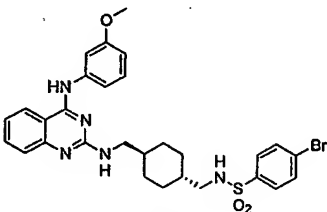
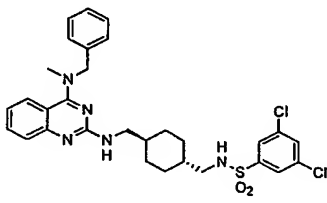
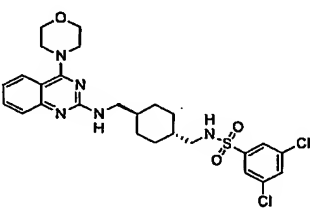
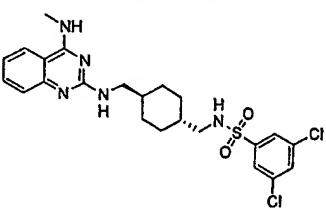
Example No.	Structure	ESI-MS	Retention Time (min)
2375	 <p>CF₃CO₂H</p>	582.4 (M + H)	4.26
2376	 <p>CF₃CO₂H</p>	536.2 (M + H)	4.06
2377	 <p>CF₃CO₂H</p>	564.2 (M + H)	4.32
2378	 <p>CF₃CO₂H</p>	566.4 (M + H)	4.11
2379	 <p>CF₃CO₂H</p>	554.2 (M + H)	4.10
2380	 <p>CF₃CO₂H</p>	614.2 (M + H)	4.26

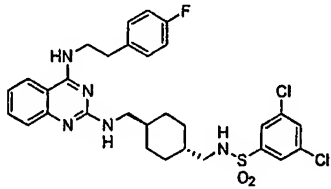
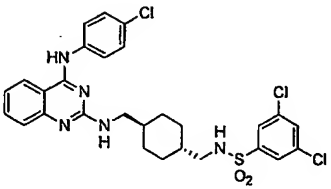
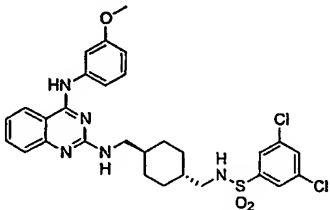
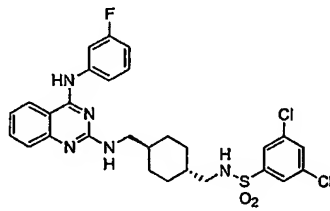
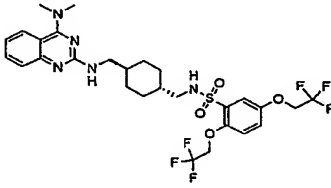
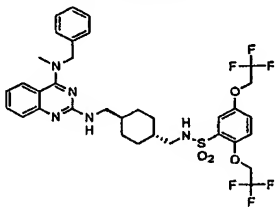
Example No.	Structure	ESI-MS	Retention Time (min)
2381	 <p>CF₃CO₂H</p>	524.4 (M + H)	3.87
2382	 <p>CF₃CO₂H</p>	568.2 (M + H)	3.87
2383	 <p>CF₃CO₂H</p>	586.2 (M + H)	4.18
2384	 <p>CF₃CO₂H</p>	614.2 (M + H)	4.45
2385	 <p>CF₃CO₂H</p>	620.4 (M + H)	4.32
2386	 <p>CF₃CO₂H</p>	468.2 (M + H)	3.20

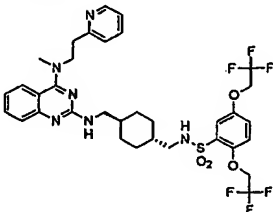
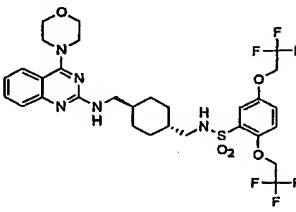
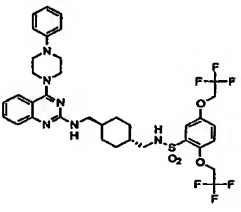
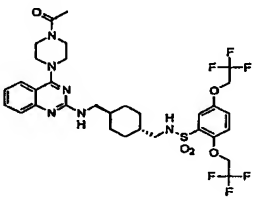
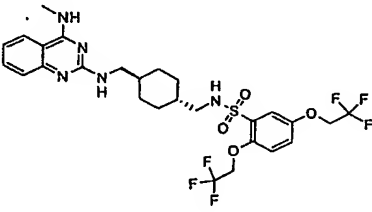
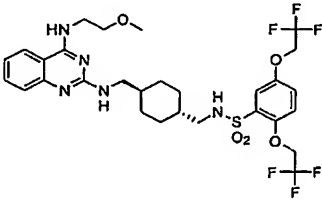
Example No.	Structure	ESI-MS	Retention Time (min)
2387	 <chem>CC1=NC2=C(N1)N=CN=C2C(S(=O)(=O)C3=CC=C(C)C)C(S(=O)(=O)C4=CC=C(C)C)C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	551.6 (M + H)	2.82
2388	 <chem>CC1=NC2=C(N1)N=CN=C2C(S(=O)(=O)C3=CC=C(C)C)C(S(=O)(=O)C4=CC=C(C)C)C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	454.0 (M + H)	3.06
2389	 <chem>CC1=NC2=C(N1)N=CN=C2C(S(=O)(=O)C3=CC=C(C)C)C(S(=O)(=O)C4=CC=C(C)C)C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	498.6 (M + H)	3.10
2390	 <chem>CC1=NC2=C(N1)N=CN=C2C(S(=O)(=O)C3=CC=C(C)C)C(S(=O)(=O)C4=CC=C(C)C)C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	484.2 (M + H)	2.76
2391	 <chem>CC1=NC2=C(N1)N=CN=C2C(S(=O)(=O)C3=CC=C(C)C)C(S(=O)(=O)C4=CC=C(C)C)C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	553.6 (M + H)	2.40
2392	 <chem>CC1=NC2=C(N1)N=CN=C2C(S(=O)(=O)C3=CC=C(C)C)C(S(=O)(=O)C4=CC=C(C)C)C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	536.4 (M + H)	3.77

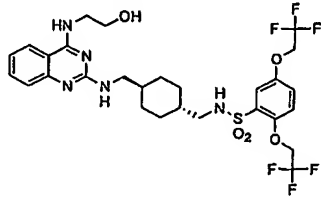
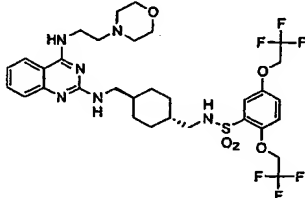
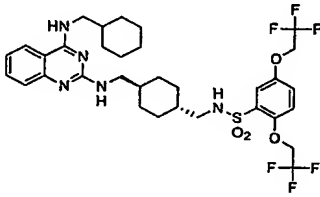
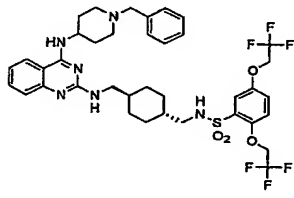
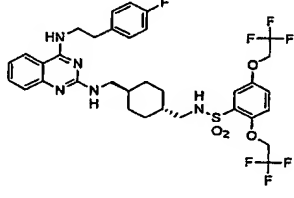
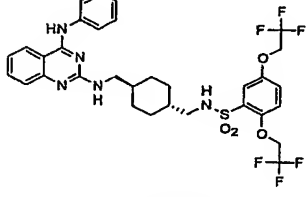
Example No.	Structure	ESI-MS	Retention Time (min)
2393	 $2\text{CF}_3\text{CO}_2\text{H}$	613.4 (M + H)	2.74
2394	 $\text{CF}_3\text{CO}_2\text{H}$	623.4 (M + H)	3.06
2395	 $\text{CF}_3\text{CO}_2\text{H}$	574.4 (M + H)	3.51
2396	 $\text{CF}_3\text{CO}_2\text{H}$	562.2 (M + H)	3.59
2397	 $2\text{CF}_3\text{CO}_2\text{H}$	548.6 (M + H)	2.48
2398	 $\text{CF}_3\text{CO}_2\text{H}$	516.4 (M + H)	3.39

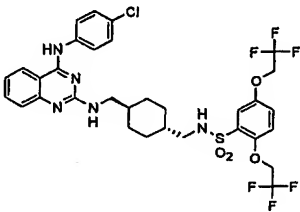
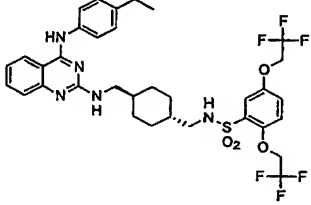
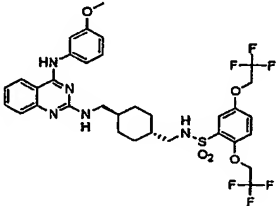
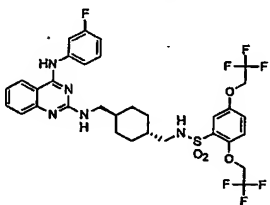
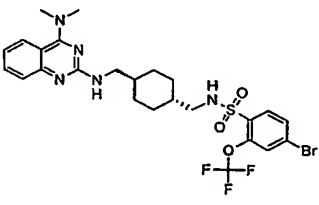
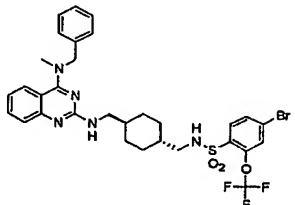
Example No.	Structure	ESI-MS	Retention Time (min)
2399	 <chem>CC1=CC=C(S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C=NC4=CC=C(NC5=CC=C(Cl)C=C5)C=C4N3)C=C1</chem> $\text{CF}_3\text{CO}_2\text{H}$	550.4 (M+H)	3.56
2400	 <chem>CC1=CC=C(S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C=NC4=CC=C(NC5=CC=C(OC)C=C5)C=C4N3)C=C1</chem> $\text{CF}_3\text{CO}_2\text{H}$	546.2 (M+H)	3.38
2401	 <chem>CC1=CC=C(S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C=NC4=CC=C(NC5=CC=C(F)C=C5)C=C4N3)C=C1</chem> $\text{CF}_3\text{CO}_2\text{H}$	534.0 (M+H)	3.43
2402	 <chem>CC1=CC=C(S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C=NC4=CC=C(NC5=CC=CC=C5)C=C4N3)C=C1</chem> $\text{CF}_3\text{CO}_2\text{H}$	608.2 (M+H)	3.75
2403	 <chem>CC1=CC=C(S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C=NC4=CC=C(NC)C=C4N3)C=C1</chem> $\text{CF}_3\text{CO}_2\text{H}$	518 (M+H)	3.22
2404	 <chem>CC1=CC=C(S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C=NC4=CC=C(NCCOC)C=C4N3)C=C1</chem> $\text{CF}_3\text{CO}_2\text{H}$	562.2 (M+H)	3.20

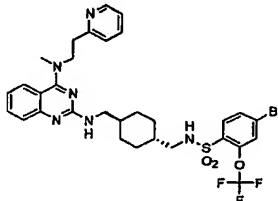
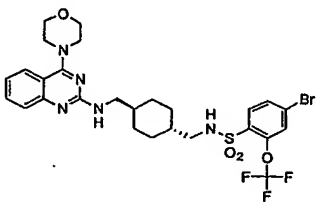
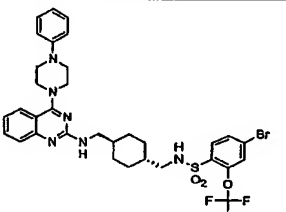
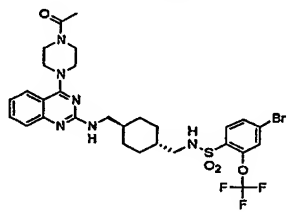
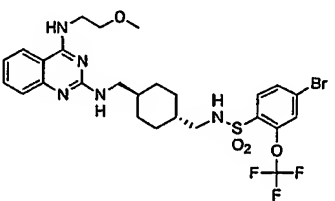
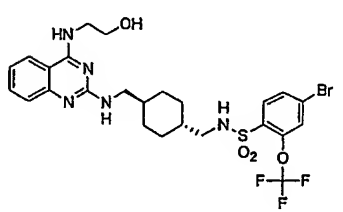
Example No.	Structure	ESI-MS	Retention Time (min)
2405	 <p>CF₃CO₂H</p>	626.0 (M + H)	3.76
2406	 <p>CF₃CO₂H</p>	614.0 (M + H)	3.72
2407	 <p>CF₃CO₂H</p>	610.0 (M + H)	3.57
2408	 <p>CF₃CO₂H</p>	598.2 (M + H)	3.97
2409	 <p>CF₃CO₂H</p>	564.2 (M + H)	3.46
2410	 <p>CF₃CO₂H</p>	508.0 (M + H)	3.44

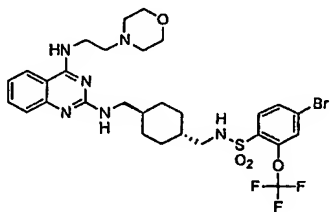
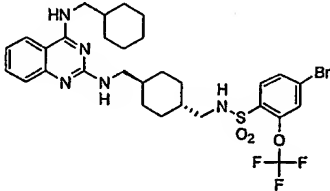
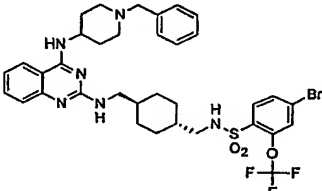
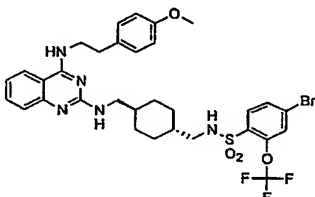
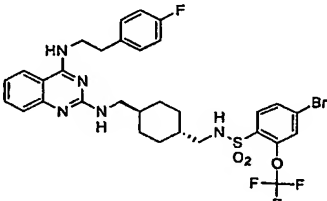
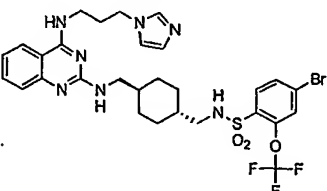
Example No.	Structure	ESI-MS	Retention Time (min)
2411	 <chem>CF3CO2H</chem>	616.2 (M + H)	3.94
2412	 <chem>CF3CO2H</chem>	604.2 (M + H)	4.51
2413	 <chem>CF3CO2H</chem>	600.2 (M + H)	4.32
2414	 <chem>CF3CO2H</chem>	588.0 (M + H)	4.38
2415	 <chem>CF3CO2H</chem>	650.2 (M + H)	4.20
2416	 <chem>CF3CO2H</chem>	726.4 (M + H)	4.52

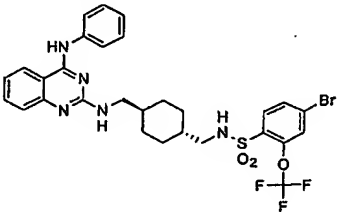
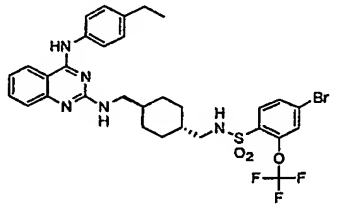
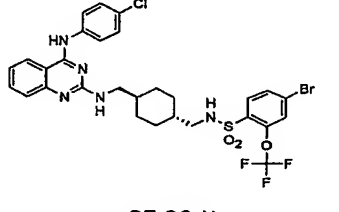
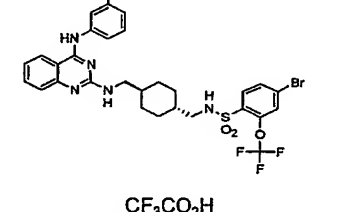
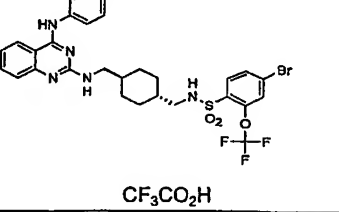
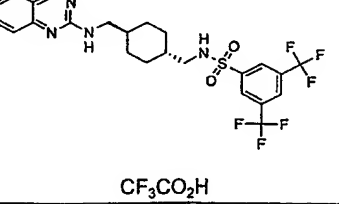
Example No.	Structure	ESI-MS	Retention Time (min)
2417	 $2\text{CF}_3\text{CO}_2\text{H}$	741.6 (M + H)	3.59
2418	 $\text{CF}_3\text{CO}_2\text{H}$	692.2 (M + H)	4.12
2419	 $2\text{CF}_3\text{CO}_2\text{H}$	767.6 (M + H)	4.59
2420	 $\text{CF}_3\text{CO}_2\text{H}$	733.4 (M + H)	3.87
2421	 $\text{CF}_3\text{CO}_2\text{H}$	636.2 (M + H)	4.08
2422	 $\text{CF}_3\text{CO}_2\text{H}$	680.2 (M + H)	4.07

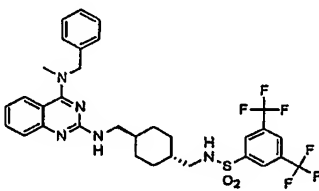
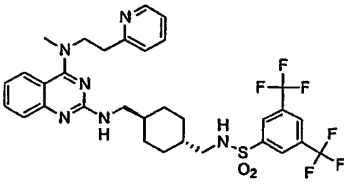
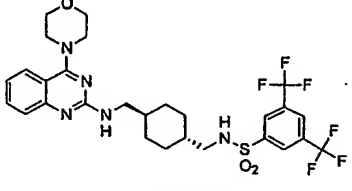
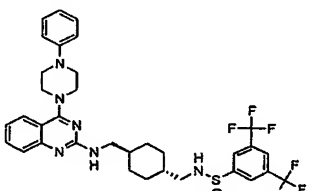
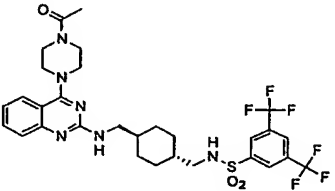
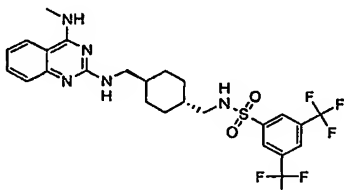
Example No.	Structure	ESI-MS	Retention Time (min)
2423	 $\text{CF}_3\text{CO}_2\text{H}$	666.0 (M + H)	3.86
2424	 $2\text{CF}_3\text{CO}_2\text{H}$	735.4 (M + H)	3.50
2425	 $\text{CF}_3\text{CO}_2\text{H}$	718.4 (M + H)	4.64
2426	 $2\text{CF}_3\text{CO}_2\text{H}$	795.6 (M + H)	3.70
2427	 $\text{CF}_3\text{CO}_2\text{H}$	744.2 (M + H)	4.43
2428	 $\text{CF}_3\text{CO}_2\text{H}$	698.0 (M + H)	4.26

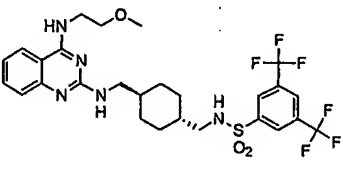
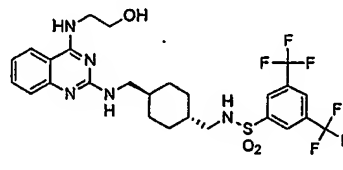
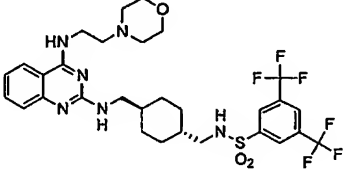
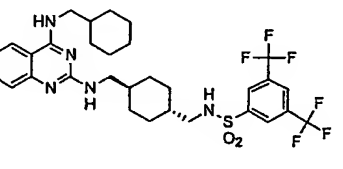
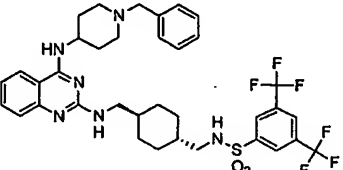
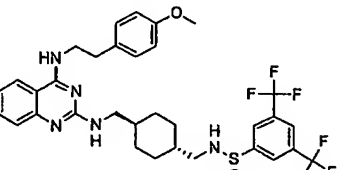
Example No.	Structure	ESI-MS	Retention Time (min)
2429	 <chem>CC(F)(F)FOC1=CC=C(C=C1)OS(=O)(=O)N[C@H]2CCCC[C@H]2CN3C(=N4C=CC=CC=C4N=C3N5C=CC=C(C=C5)NC6=CC=CC=C6Cl)C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	732.4 (M + H)	4.37
2430	 <chem>CC(F)(F)FOC1=CC=C(C=C1)OS(=O)(=O)N[C@H]2CCCC[C@H]2CN3C(=N4C=CC=CC=C4N=C3N5C=CC=C(C=C5)NC6=CC=C(C=C6)CC)C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	726.4 (M + H)	4.52
2431	 <chem>CC(F)(F)FOC1=CC=C(C=C1)OS(=O)(=O)N[C@H]2CCCC[C@H]2CN3C(=N4C=CC=CC=C4N=C3N5C=CC=C(C=C5)NC6=CC=C(C=C6)OC)C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	728.4 (M + H)	4.36
2432	 <chem>CC(F)(F)FOC1=CC=C(C=C1)OS(=O)(=O)N[C@H]2CCCC[C@H]2CN3C(=N4C=CC=CC=C4N=C3N5C=CC=C(C=C5)NC6=CC=C(C=C6)F)C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	716.4 (M + H)	4.32
2433	 <chem>CC(F)(F)FOC1=CC=C(C=C1)OS(=O)(=O)N[C@H]2CCCC[C@H]2CN3C(=N4C=CC=CC=C4N=C3N5C=CC=C(C=C5)NC6=CC=C(C=C6)N(C)C)C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	616.0 (M + H)	4.22
2434	 <chem>CC(F)(F)FOC1=CC=C(C=C1)OS(=O)(=O)N[C@H]2CCCC[C@H]2CN3C(=N4C=CC=CC=C4N=C3N5C=CC=C(C=C5)NC6=CC=C(C=C6)CC7=CC=C(C=C7)Br)C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	692.0 (M + H)	4.57

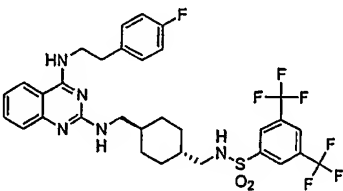
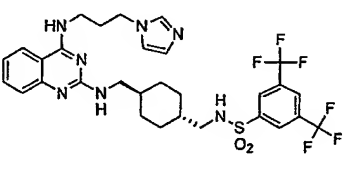
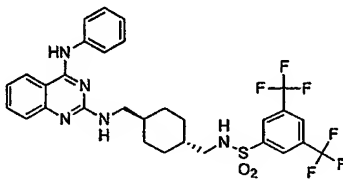
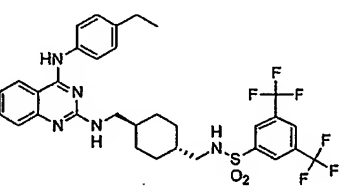
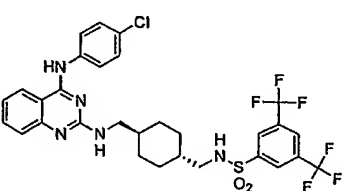
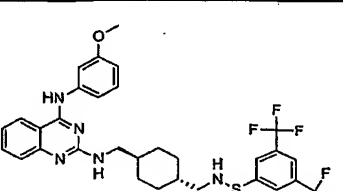
Example No.	Structure	ESI-MS	Retention Time (min)
2435	 $2\text{CF}_3\text{CO}_2\text{H}$	707.2 (M + H)	3.64
2436	 $\text{CF}_3\text{CO}_2\text{H}$	658.2 (M + H)	4.15
2437	 $\text{CF}_3\text{CO}_2\text{H}$	733.2 (M + H)	4.68
2438	 $\text{CF}_3\text{CO}_2\text{H}$	699.2 (M + H)	3.88
2439	 $\text{CF}_3\text{CO}_2\text{H}$	646.4 (M + H)	4.08
2440	 $\text{CF}_3\text{CO}_2\text{H}$	632.4 (M + H)	3.86

Example No.	Structure	ESI-MS	Retention Time (min)
2441	 $2\text{CF}_3\text{CO}_2\text{H}$	701.4 (M + H)	3.51
2442	 $\text{CF}_3\text{CO}_2\text{H}$	684.2 (M + H)	4.75
2443	 $2\text{CF}_3\text{CO}_2\text{H}$	761.2 (M + H)	3.74
2444	 $\text{CF}_3\text{CO}_2\text{H}$	722.2 (M + H)	4.59
2445	 $\text{CF}_3\text{CO}_2\text{H}$	710.2 (M + H)	4.60
2446	 $2\text{CF}_3\text{CO}_2\text{H}$	696.2 (M + H)	3.53

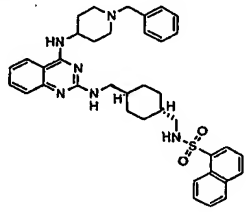
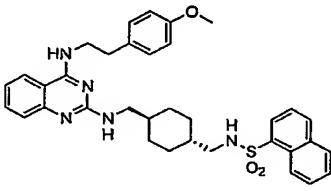
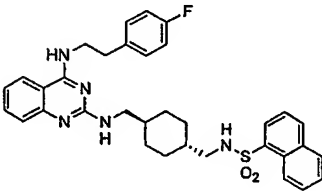
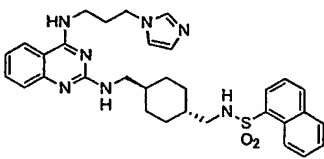
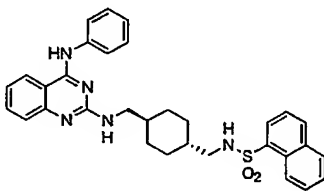
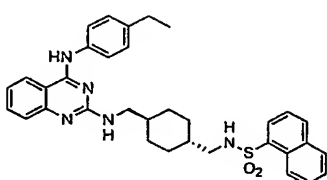
Example No.	Structure	ESI-MS	Retention Time (min)
2447	 <chem>Brc1ccc(cc1OS(=O)(=O)N[C@H]2CCCC[C@H]2C3=NC4=CC=CC=C4N=C3N5C(=NC6=CC=CC=C6N5)C(=N4)Nc7ccccc7</chem> $\text{CF}_3\text{CO}_2\text{H}$	664.2 (M + H)	4.39
2448	 <chem>CCc1ccc(cc1)Nc2nc3c(nc4c2nc5ccccc54)C(=N3)N[C@H]6CCCC[C@H]6C(=N1)S(=O)(=O)N1C=CC(OC(F)(F)F)=CC=C1Br</chem> $\text{CF}_3\text{CO}_2\text{H}$	692.0 (M + H)	4.65
2449	 <chem>Clc1ccc(cc1)Nc2nc3c(nc4c2nc5ccccc54)C(=N3)N[C@H]6CCCC[C@H]6C(=N1)S(=O)(=O)N1C=CC(OC(F)(F)F)=CC=C1Br</chem> $\text{CF}_3\text{CO}_2\text{H}$	698.0 (M + H)	4.59
2450	 <chem>COc1ccc(cc1)Nc2nc3c(nc4c2nc5ccccc54)C(=N3)N[C@H]6CCCC[C@H]6C(=N1)S(=O)(=O)N1C=CC(OC(F)(F)F)=CC=C1Br</chem> $\text{CF}_3\text{CO}_2\text{H}$	694.2 (M + H)	4.42
2451	 <chem>Fc1ccc(cc1)Nc2nc3c(nc4c2nc5ccccc54)C(=N3)N[C@H]6CCCC[C@H]6C(=N1)S(=O)(=O)N1C=CC(OC(F)(F)F)=CC=C1Br</chem> $\text{CF}_3\text{CO}_2\text{H}$	682.2 (M + H)	4.42
2452	 <chem>CN(C)c1ccc(cc1)Nc2nc3c(nc4c2nc5ccccc54)C(=N3)N[C@H]6CCCC[C@H]6C(=N1)S(=O)(=O)N1C=CC(F)(F)F=CC=C1C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	590.2 (M + H)	4.28

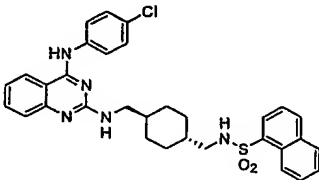
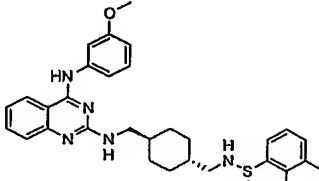
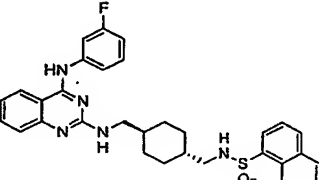
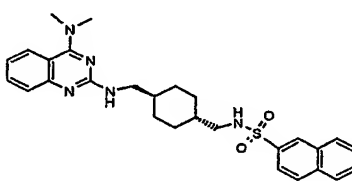
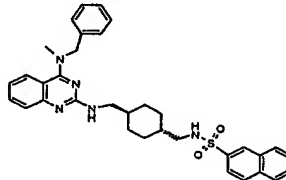
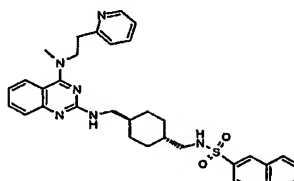
Example No.	Structure	ESI-MS	Retention Time (min)
2453	 $\text{CF}_3\text{CO}_2\text{H}$	666.2 (M + H)	4.61
2454	 $2\text{CF}_3\text{CO}_2\text{H}$	681.2 (M + H)	3.72
2455	 $\text{CF}_3\text{CO}_2\text{H}$	632.4 (M + H)	4.21
2456	 $2\text{CF}_3\text{CO}_2\text{H}$	707.2 (M + H)	4.70
2457	 $\text{CF}_3\text{CO}_2\text{H}$	673.2 (M + H)	3.94
2458	 $\text{CF}_3\text{CO}_2\text{H}$	576.2 (M + H)	4.16

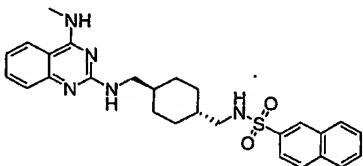
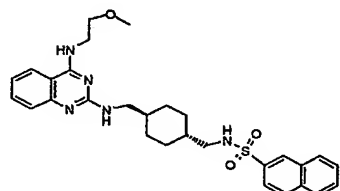
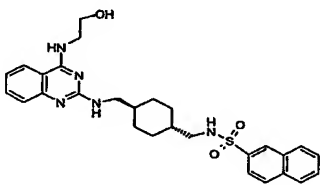
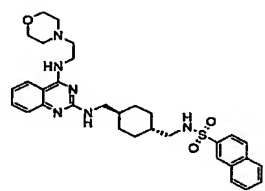
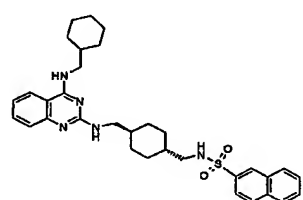
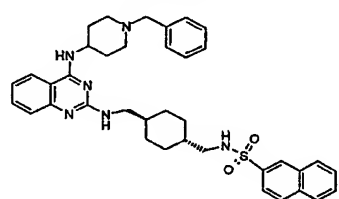
Example No.	Structure	ESI-MS	Retention Time (min)
2459	 <chem>COCCNc1nc2c(ncn2C1CCCC1)nc3ccccc3</chem> <chem>CF3CO2H</chem>	620.4 (M + H)	4.19
2460	 <chem>CCOCCNc1nc2c(ncn2C1CCCC1)nc3ccccc3</chem> <chem>CF3CO2H</chem>	606.6 (M + H)	3.94
2461	 <chem>C1CCN(C1)CCNc2nc3c(ncn3C2CCCC2)nc4ccccc4</chem> <chem>2CF3CO2H</chem>	675.4 (M + H)	3.59
2462	 <chem>C1CCCCC1Nc2nc3c(ncn3C2CCCC2)nc4ccccc4</chem> <chem>CF3CO2H</chem>	658.6 (M + H)	4.82
2463	 <chem>c1ccc(cc1)CN2CCCCC2Nc3nc4c(ncn4C3CCCC3)nc5ccccc5</chem> <chem>2CF3CO2H</chem>	735.4 (M + H)	3.82
2464	 <chem>COc1ccc(cc1)CCNc2nc3c(ncn3C2CCCC2)nc4ccccc4</chem> <chem>CF3CO2H</chem>	696.0 (M + H)	4.56

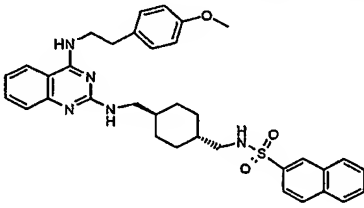
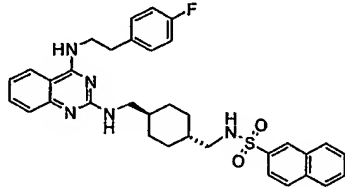
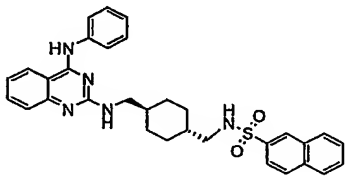
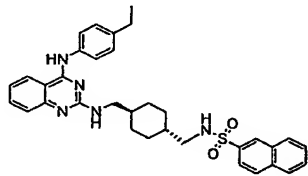
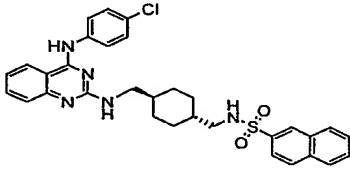
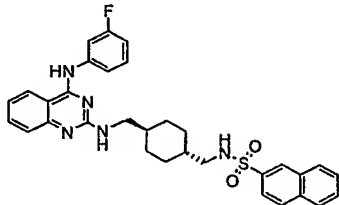
Example No.	Structure	ESI-MS	Retention Time (min)
2465	 <chem>CF3CO2H</chem>	684.4 (M + H)	4.61
2466	 <chem>2CF3CO2H</chem>	670.2 (M + H)	3.56
2467	 <chem>CF3CO2H</chem>	638.2 (M + H)	4.43
2468	 <chem>CF3CO2H</chem>	666.2 (M + H)	4.68
2469	 <chem>CF3CO2H</chem>	672.2 (M + H)	4.60
2470	 <chem>CF3CO2H</chem>	668.2 (M + H)	4.44

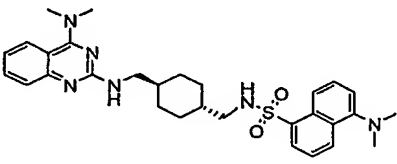
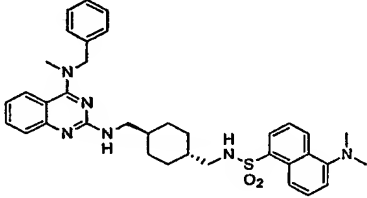
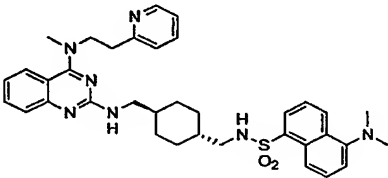
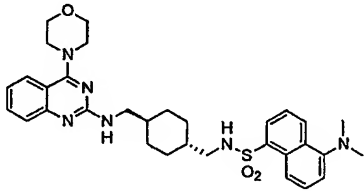
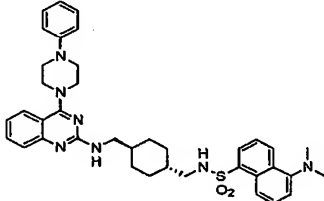
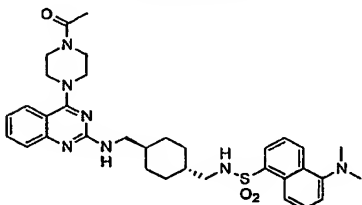
Example No.	Structure	ESI-MS	Retention Time (min)
2471	 <chem>FC1=CC=C(C=C1)Nc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5cc(C(F)(F)F)cc(C(F)(F)F)c5</chem> $\text{CF}_3\text{CO}_2\text{H}$	656.4 (M + H)	4.47
2472	 <chem>CN1CCCC1Cc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5cc(C(F)(F)F)cc(C(F)(F)F)c5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	595.4 (M + H)	3.32
2473	 <chem>COCNc1nc2ccccc2n1CNC3CCCCC3NS(=O)(=O)c4cc5ccccc5cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	534.0 (M + H)	3.81
2474	 <chem>OCCNc1nc2ccccc2n1CNC3CCCCC3NS(=O)(=O)c4cc5ccccc5cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	520.4 (M + H)	3.56
2475	 <chem>C1CCN(CC1)CCNc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5cc(C(F)(F)F)cc(C(F)(F)F)c5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	589.2 (M + H)	3.25
2476	 <chem>C1CCCCC1CNc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5cc(C(F)(F)F)cc(C(F)(F)F)c5</chem> $\text{CF}_3\text{CO}_2\text{H}$	572.4 (M + H)	4.47

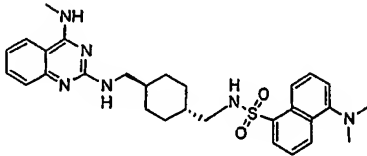
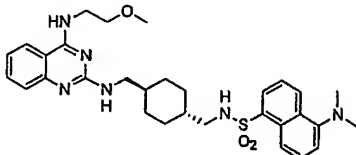
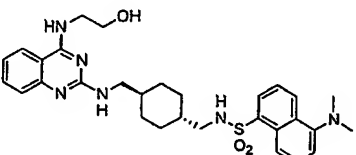
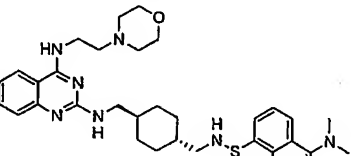
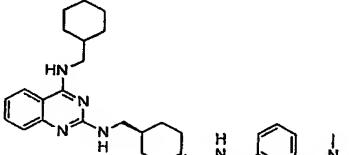
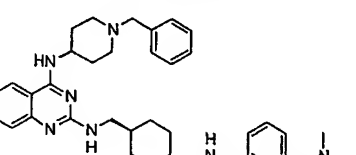
Example No.	Structure	ESI-MS	Retention Time (min)
2477	 $2CF_3CO_2H$	649.4 (M + H)	3.50
2478	 CF_3CO_2H	610.4 (M + H)	4.26
2479	 CF_3CO_2H	598.2 (M + H)	4.30
2480	 $2CF_3CO_2H$	584.4 (M + H)	3.29
2481	 CF_3CO_2H	552.6 (M + H)	4.11
2482	 CF_3CO_2H	580.6 (M + H)	4.40

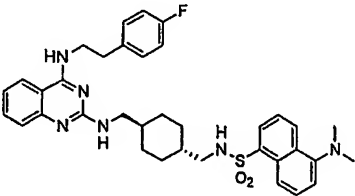
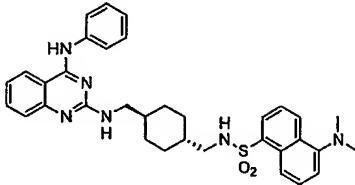
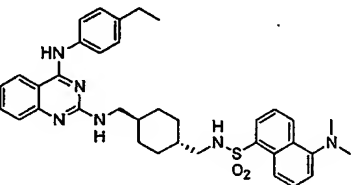
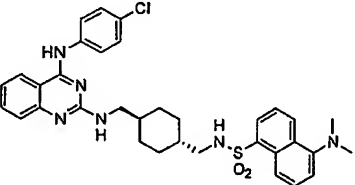
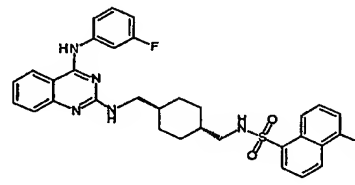
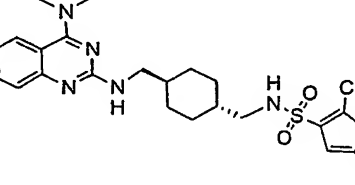
Example No.	Structure	ESI-MS	Retention Time (min)
2483	 <chem>Clc1ccc(Nc2nc3ccccc3n2NC[C@H]4CCCC[C@H]4NS(=O)(=O)c5cc6ccccc6cc5)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	586.2 (M + H)	4.30
2484	 <chem>COc1ccc(Nc2nc3ccccc3n2NC[C@H]4CCCC[C@H]4NS(=O)(=O)c5cc6ccccc6cc5)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	582.4 (M + H)	4.14
2485	 <chem>Fc1ccc(Nc2nc3ccccc3n2NC[C@H]4CCCC[C@H]4NS(=O)(=O)c5cc6ccccc6cc5)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	570.2 (M + H)	4.14
2486	 <chem>CN1C=NC2=C(N1)C=CC=C2NC[C@H]3CCCC[C@H]3NS(=O)(=O)c4cc5ccccc5cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	504.2 (M + H)	3.94
2487	 <chem>CN(Cc1ccccc1)C2=NC3=CC=CC=C3N=C2NC[C@H]4CCCC[C@H]4NS(=O)(=O)c5cc6ccccc6cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	580.6 (M + H)	4.34
2488	 <chem>CN(Cc1ccccc1)C2=NC3=CC=CC=C3N=C2NC[C@H]4CCCC[C@H]4NS(=O)(=O)c5cc6ccccc6cc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	595.2 (M + H)	3.41

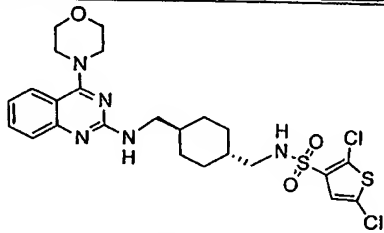
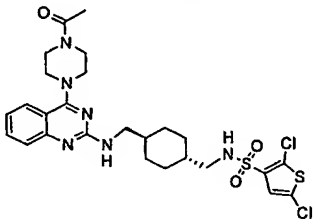
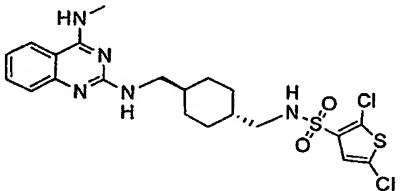
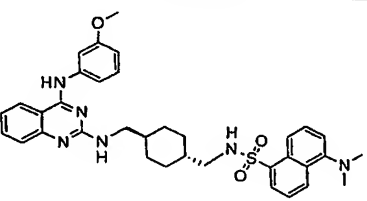
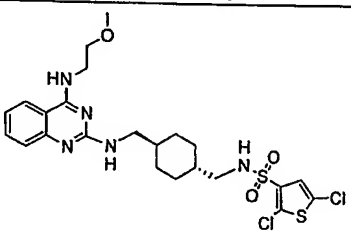
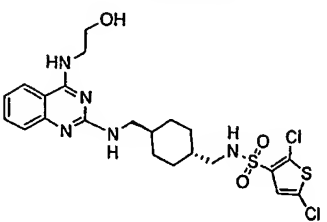
Example No.	Structure	ESI-MS	Retention Time (min)
2489	 <p>CF₃CO₂H</p>	490.2 (M + H)	3.84
2490	 <p>CF₃CO₂H</p>	534.2 (M + H)	3.84
2491	 <p>CF₃CO₂H</p>	520.4 (M + H)	3.60
2492	 <p>2CF₃CO₂H</p>	589.2 (M + H)	3.29
2493	 <p>CF₃CO₂H</p>	572.4 (M + H)	4.51
2494	 <p>2CF₃CO₂H</p>	649.4 (M + H)	3.52

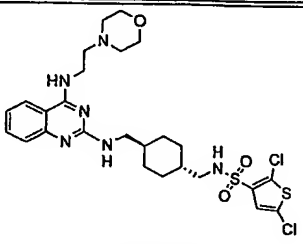
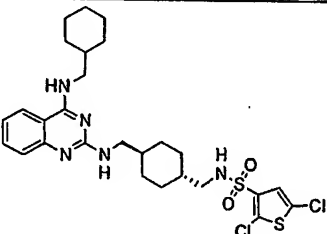
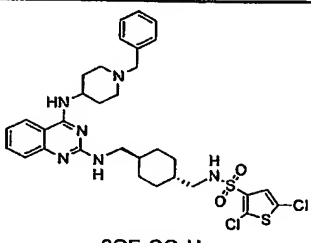
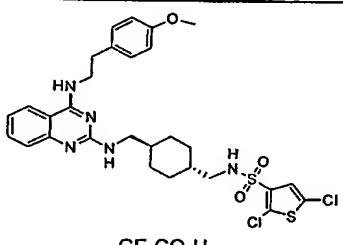
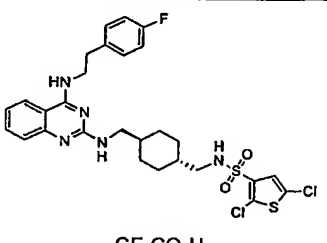
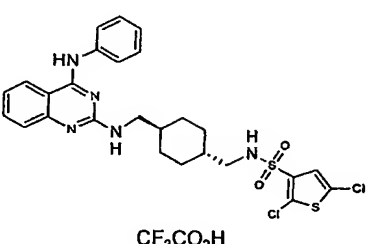
Example No.	Structure	ESI-MS	Retention Time (min)
2495	 <chem>COc1ccc(cc1)CNc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5ccc6ccccc65</chem> $\text{CF}_3\text{CO}_2\text{H}$	610.2 (M + H)	4.29
2496	 <chem>Fc1ccc(cc1)CNc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5ccc6ccccc65</chem> $\text{CF}_3\text{CO}_2\text{H}$	598.2 (M + H)	4.34
2497	 <chem>c1ccc(cc1)Nc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5ccc6ccccc65</chem> $\text{CF}_3\text{CO}_2\text{H}$	552.6 (M + H)	4.13
2498	 <chem>CCc1ccc(cc1)Nc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5ccc6ccccc65</chem> $\text{CF}_3\text{CO}_2\text{H}$	580.6 (M + H)	4.37
2499	 <chem>Clc1ccc(cc1)Nc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5ccc6ccccc65</chem> $\text{CF}_3\text{CO}_2\text{H}$	586.2 (M + H)	4.30
2500	 <chem>Fc1cccc(c1)Nc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5ccc6ccccc65</chem> $\text{CF}_3\text{CO}_2\text{H}$	570.2 (M + H)	4.18

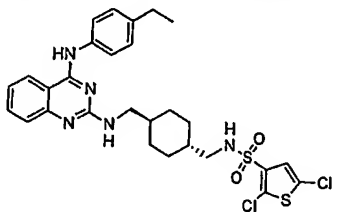
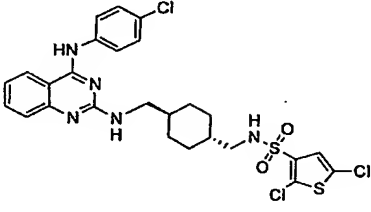
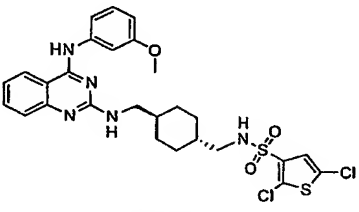
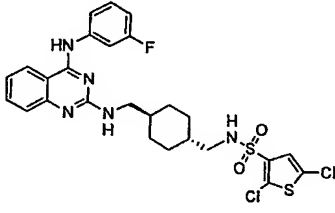
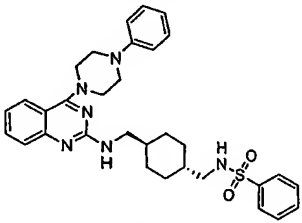
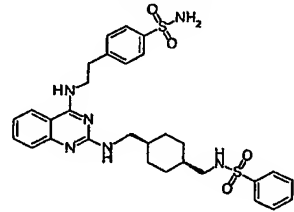
Example No.	Structure	ESI-MS	Retention Time (min)
2501	 <chem>CN(C)Cc1nc2ccccc2n1CNC3CCCCC3NS(=O)(=O)c4ccc(N(C)C)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	547.4 (M + H)	3.69
2502	 <chem>CN(C)Cc1nc2ccccc2n1C=Cc3ccccc3CNC4CCCCC4NS(=O)(=O)c5ccc(N(C)C)cc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	623.4 (M + H)	4.10
2503	 <chem>CN(C)Cc1nc2ccccc2n1CNC3CCCCC3NS(=O)(=O)c4ccc(N(C)C)cc4</chem> $3\text{CF}_3\text{CO}_2\text{H}$	638.2 (M + H)	3.20
2504	 <chem>CN(C)Cc1nc2ccccc2n1CNC3CCCCC3NS(=O)(=O)c4ccc(N(C)C)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	589.2 (M + H)	3.62
2505	 <chem>CN(C)Cc1nc2ccccc2n1CNC3CCCCC3NS(=O)(=O)c4ccc(N(C)C)cc4</chem> $3\text{CF}_3\text{CO}_2\text{H}$	664.4 (M + H)	4.25
2506	 <chem>CC(=O)N1CCN(C1)Cc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5ccc(N(C)C)cc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	630.4 (M + H)	3.35

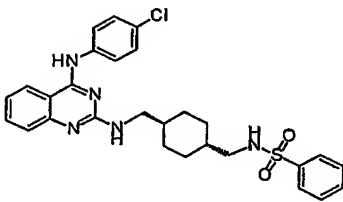
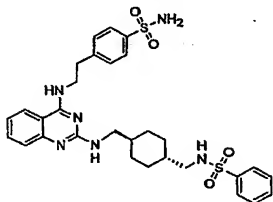
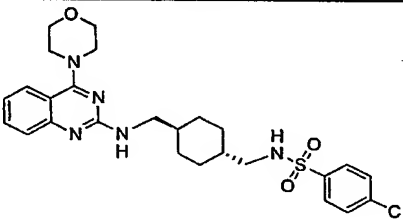
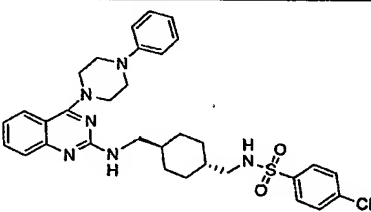
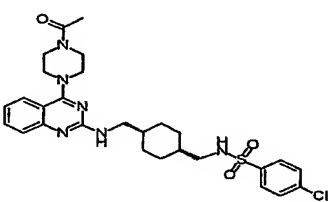
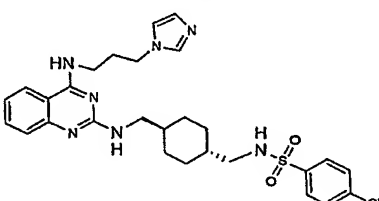
Example No.	Structure	ESI-MS	Retention Time (min)
2507	 <chem>CC1=CC=C(C=C1)S(=O)(=O)NCC2=CC=CC=C2N3C=NC4=CC=CC=C4N3C2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	533.2 (M + H)	3.57
2508	 <chem>COCCN1C=NC2=CC=CC=C2N1C3=CC=CC=C3N3C=CC(=C3)S(=O)(=O)NCC4=CC=CC=C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	577.6 (M + H)	3.58
2509	 <chem>CC1=CC=C(C=C1)S(=O)(=O)NCC2=CC=CC=C2N3C=NC4=CC=CC=C4N3C2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	563.2 (M + H)	3.28
2510	 <chem>CC1=CC=C(C=C1)S(=O)(=O)NCC2=CC=CC=C2N3C=NC4=CC=CC=C4N3C2</chem> $3\text{CF}_3\text{CO}_2\text{H}$	632.6 (M + H)	3.06
2511	 <chem>CC1=CC=C(C=C1)S(=O)(=O)NCC2=CC=CC=C2N3C=NC4=CC=CC=C4N3C2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	615.4 (M + H)	4.30
2512	 <chem>CC1=CC=C(C=C1)S(=O)(=O)NCC2=CC=CC=C2N3C=NC4=CC=CC=C4N3C2</chem> $3\text{CF}_3\text{CO}_2\text{H}$	692.2 (M + H)	3.38

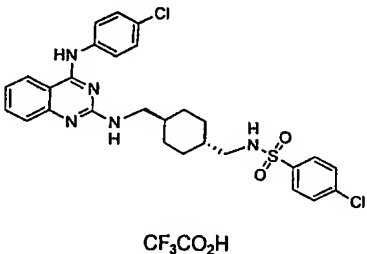
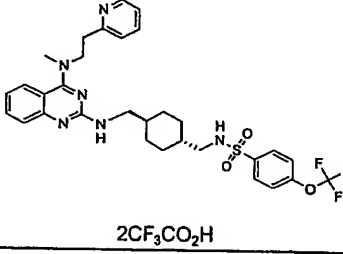
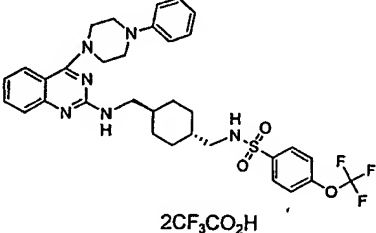
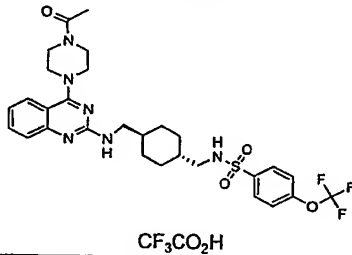
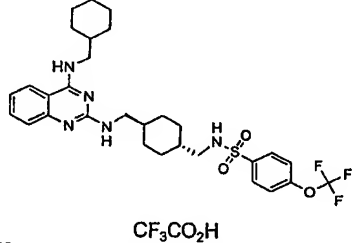
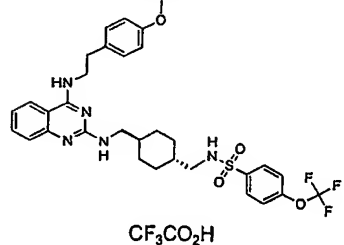
Example No.	Structure	ESI-MS	Retention Time (min)
2513	 <chem>CC1=CC=C(C=C1)S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C=NC4=CC=CC=C4N3C5=CC=C(C=C5)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	641.4 (M + H)	4.13
2514	 <chem>CC1=CC=C(C=C1)S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C=NC4=CC=CC=C4N3C5=CC=CC=C5N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	595.4 (M + H)	3.89
2515	 <chem>CC1=CC=C(C=C1)S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C=NC4=CC=CC=C4N3C5=CC=C(C=C5)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	623.4 (M + H)	4.20
2516	 <chem>CC1=CC=C(C=C1)S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C=NC4=CC=CC=C4N3C5=CC=C(C=C5)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	629.2 (M + H)	4.15
2517	 <chem>CC1=CC=C(C=C1)S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C=NC4=CC=CC=C4N3C5=CC=C(C=C5)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	613.2 (M + H)	4.02
2518	 <chem>CC1=CC=C(C=C1)S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C=NC4=CC=CC=C4N3C5=CC=C(C=C5)N</chem> $\text{CF}_3\text{CO}_2\text{H}$	528.2 (M + H)	4.03

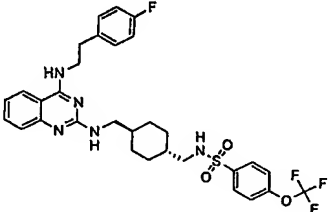
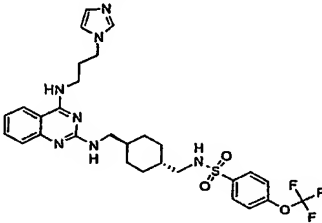
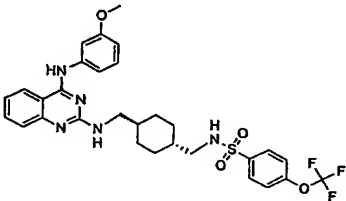
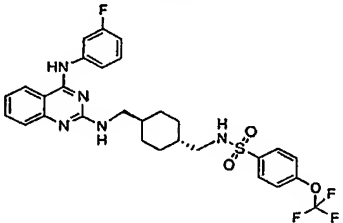
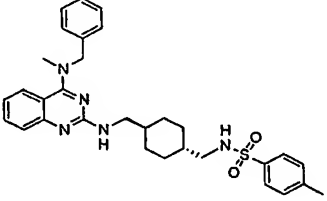
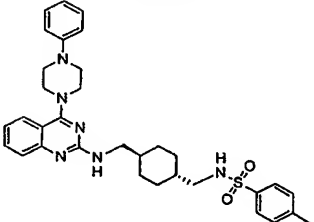
Example No.	Structure	ESI-MS	Retention Time (min)
2519	 <chem>CC1(CCN(C1)c2ccccc2N3C4CCOCC4=N3)CCN5C(=O)S(=O)(=O)C5Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	570.2 (M + H)	3.96
2520	 <chem>CC1(CCN(C1)c2ccccc2N3C4CCOCC4=N3)CCN5C(=O)S(=O)(=O)C5Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	611.0 (M + H)	3.69
2521	 <chem>CC1(CCN(C1)c2ccccc2N3C4CCOCC4=N3)CCN5C(=O)S(=O)(=O)C5Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	514.2 (M + H)	3.94
2522	 <chem>COc1ccc(NC2=NC3C(=N2)c4ccccc4N3)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	625.4 (M + H)	3.94
2523	 <chem>COCCN1=NC2C(=N1)c3ccccc3N2</chem> $\text{CF}_3\text{CO}_2\text{H}$	558.2 (M + H)	3.96
2524	 <chem>OCCN1=NC2C(=N1)c3ccccc3N2</chem> $\text{CF}_3\text{CO}_2\text{H}$	544.2 (M + H)	3.67

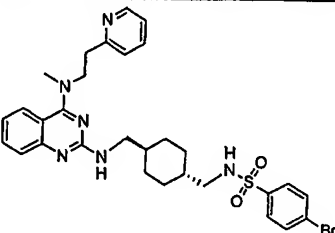
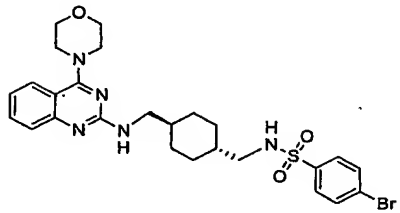
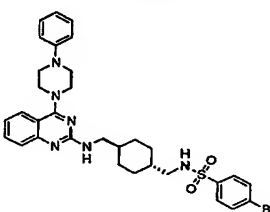
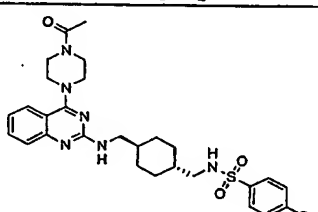
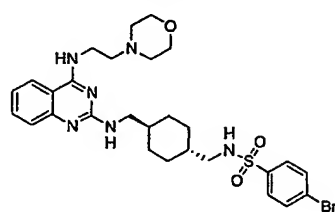
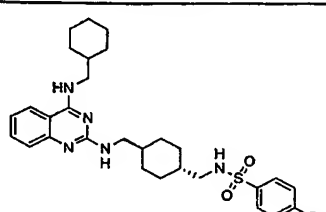
Example No.	Structure	ESI-MS	Retention Time (min)
2525	 $2\text{CF}_3\text{CO}_2\text{H}$	613.2 (M + H)	3.31
2526	 $\text{CF}_3\text{CO}_2\text{H}$	596.2 (M + H)	4.69
2527	 $2\text{CF}_3\text{CO}_2\text{H}$	673.4 (M + H)	3.57
2528	 $\text{CF}_3\text{CO}_2\text{H}$	634.4 (M + H)	4.41
2529	 $\text{CF}_3\text{CO}_2\text{H}$	622.2 (M + H)	4.45
2530	 $\text{CF}_3\text{CO}_2\text{H}$	576 (M + H)	4.25

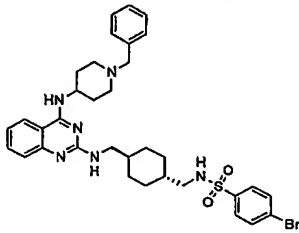
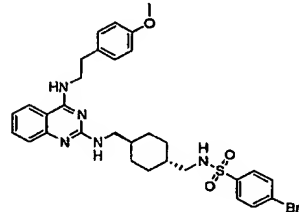
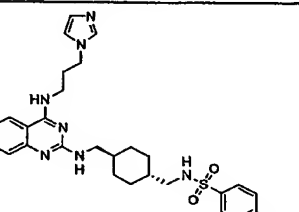
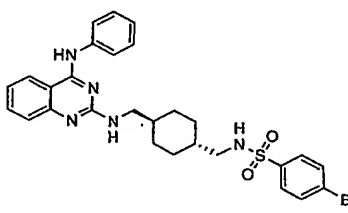
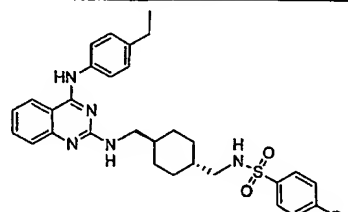
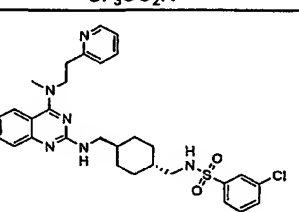
Example No.	Structure	ESI-MS	Retention Time (min)
2531	 <chem>CC1=CC=C(NC2=NC3=CC=CC=C3N2CNC4CCCCC4NS(=O)(=O)C5=CC(=C(S5)Cl)Cl)C6=CC=CC=C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	604.4 (M + H)	4.52
2532	 <chem>ClC1=CC=C(NC2=NC3=CC=CC=C3N2CNC4CCCCC4NS(=O)(=O)C5=CC(=C(S5)Cl)Cl)C6=CC=CC=C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	610.2 (M + H)	4.40
2533	 <chem>COc1ccc(NC2=NC3=CC=CC=C3N2CNC4CCCCC4NS(=O)(=O)C5=CC(=C(S5)Cl)Cl)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	606.4 (M + H)	4.29
2534	 <chem>Fc1cccc(NC2=NC3=CC=CC=C3N2CNC4CCCCC4NS(=O)(=O)C5=CC(=C(S5)Cl)Cl)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	594.2 (M + H)	4.27
2535	 <chem>c1ccc(NC2=NC3=CC=CC=C3N2CNC4CCCCC4NS(=O)(=O)c5ccccc5)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	571.8 (M + H)	4.99
2536	 <chem>O=C(N)Cc1ccc(cc1)Nc2nc3ccccc3n2CNC4CCCCC4NC(=O)c5ccccc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	609.8 (M + H)	4.43

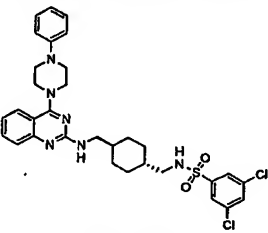
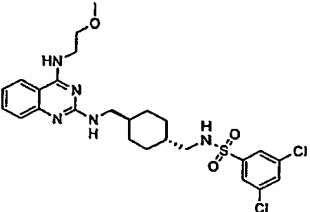
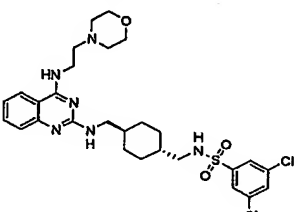
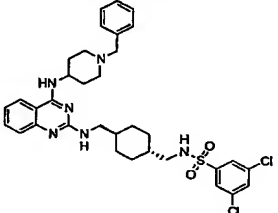
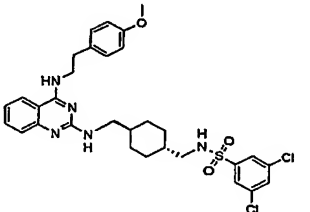
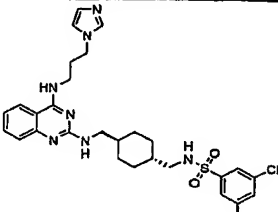
Example No.	Structure	ESI-MS	Retention Time (min)
2537	 $\text{CF}_3\text{CO}_2\text{H}$	536.4 (M + H)	4.86
2538	 $\text{CF}_3\text{CO}_2\text{H}$	564.6 (M + H)	5.13
2539	 $\text{CF}_3\text{CO}_2\text{H}$	530.6 (M + H)	4.65
2540	 $2\text{CF}_3\text{CO}_2\text{H}$	605.6 (M + H)	5.21
2541	 $\text{CF}_3\text{CO}_2\text{H}$	571.6 (M + H)	4.45
2542	 $2\text{CF}_3\text{CO}_2\text{H}$	568.8 (M + H)	4.09

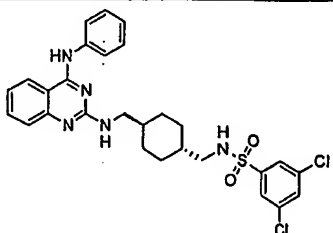
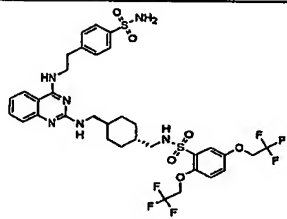
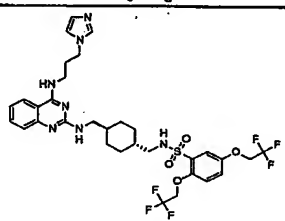
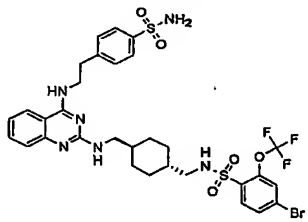
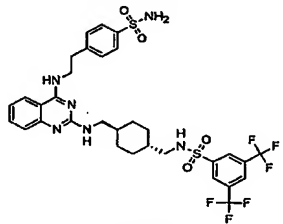
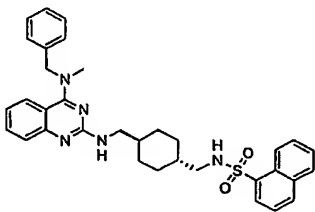
Example No.	Structure	ESI-MS	Retention Time (min)
2543	 CF ₃ CO ₂ H	570.6 (M + H)	5.11
2544	 2CF ₃ CO ₂ H	629.6 (M + H)	4.37
2545	 2CF ₃ CO ₂ H	655.6 (M + H)	5.35
2546	 CF ₃ CO ₂ H	621.8 (M + H)	4.63
2547	 CF ₃ CO ₂ H	606.8 (M + H)	5.45
2548	 CF ₃ CO ₂ H	644.6 (M + H)	5.21

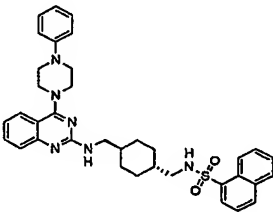
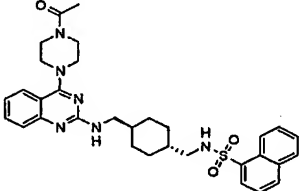
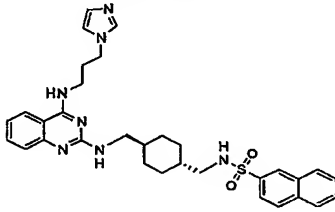
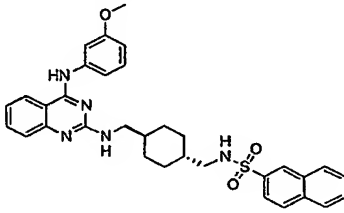
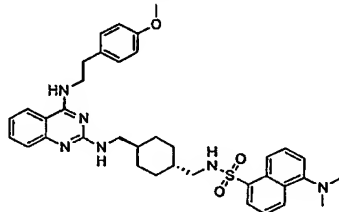
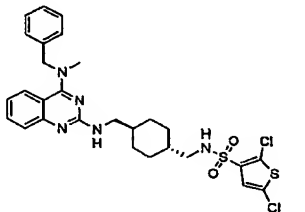
Example No.	Structure	ESI-MS	Retention Time (min)
2549	 $\text{CF}_3\text{CO}_2\text{H}$	632.6 (M + H)	5.25
2550	 $2\text{CF}_3\text{CO}_2\text{H}$	618.6 (M + H)	4.29
2551	 $\text{CF}_3\text{CO}_2\text{H}$	616.6 (M + H)	5.14
2552	 $\text{CF}_3\text{CO}_2\text{H}$	604.6 (M + H)	5.13
2553	 $\text{CF}_3\text{CO}_2\text{H}$	544.6 (M + H)	5.03
2554	 $2\text{CF}_3\text{CO}_2\text{H}$	585.6 (M + H)	5.13

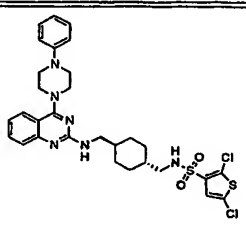
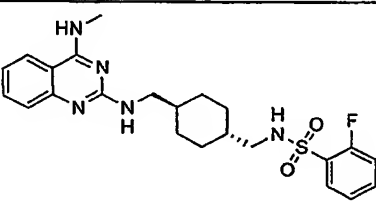
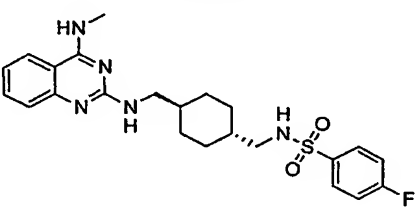
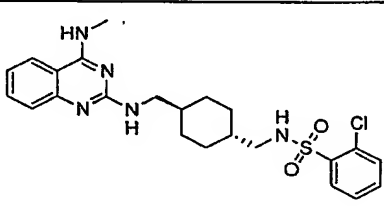
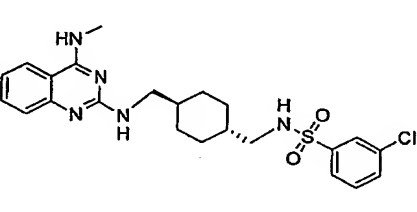
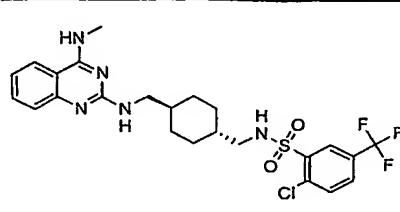
Example No.	Structure	ESI-MS	Retention Time (min)
2555	 $2\text{CF}_3\text{CO}_2\text{H}$	623.6 (M + H)	4.25
2556	 $\text{CF}_3\text{CO}_2\text{H}$	574.6 (M + H)	4.73
2557	 $2\text{CF}_3\text{CO}_2\text{H}$	649.0 (M + H)	5.25
2558	 $\text{CF}_3\text{CO}_2\text{H}$	615.0 (M + H)	4.51
2559	 $2\text{CF}_3\text{CO}_2\text{H}$	617.4 (M + H)	4.15
2560	 $\text{CF}_3\text{CO}_2\text{H}$	600.6 (M + H)	5.37

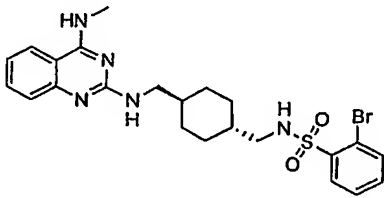
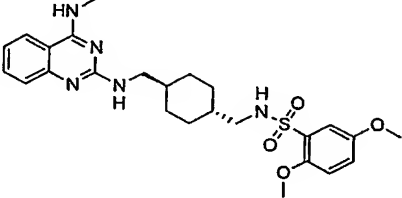
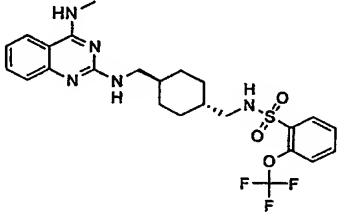
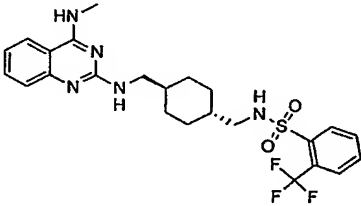
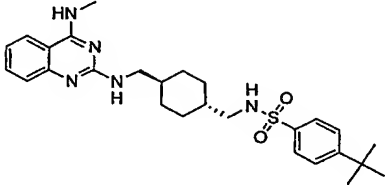
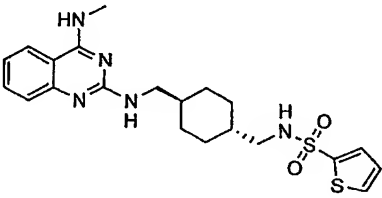
Example No.	Structure	ESI-MS	Retention Time (min)
2561	 $2\text{CF}_3\text{CO}_2\text{H}$	677.0 (M + H)	4.45
2562	 $\text{CF}_3\text{CO}_2\text{H}$	638.6 (M + H)	5.18
2563	 $2\text{CF}_3\text{CO}_2\text{H}$	612.6 (M + H)	4.16
2564	 $\text{CF}_3\text{CO}_2\text{H}$	580.0 (M + H)	5.01
2565	 $\text{CF}_3\text{CO}_2\text{H}$	608.0 (M + H)	5.26
2566	 $2\text{CF}_3\text{CO}_2\text{H}$	613.6 (M + H)	4.44

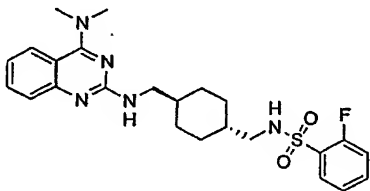
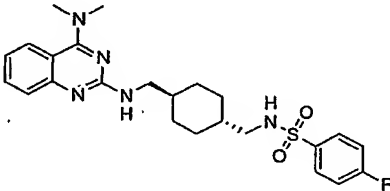
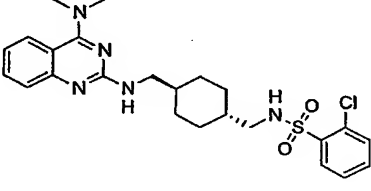
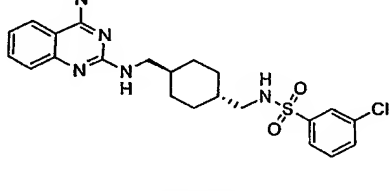
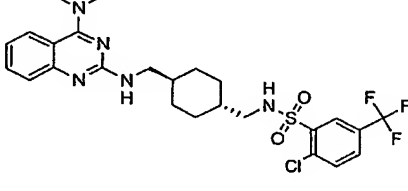
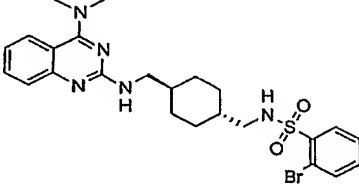
Example No.	Structure	ESI-MS	Retention Time (min)
2567	 $2\text{CF}_3\text{CO}_2\text{H}$	639.6 (M + H)	5.48
2568	 $\text{CF}_3\text{CO}_2\text{H}$	552.6 (M + H)	4.92
2569	 $2\text{CF}_3\text{CO}_2\text{H}$	607.8 (M + H)	4.33
2570	 $2\text{CF}_3\text{CO}_2\text{H}$	667.4 (M + H)	4.67
2571	 $\text{CF}_3\text{CO}_2\text{H}$	628.6 (M + H)	5.29
2572	 $2\text{CF}_3\text{CO}_2\text{H}$	602.6 (M + H)	4.35

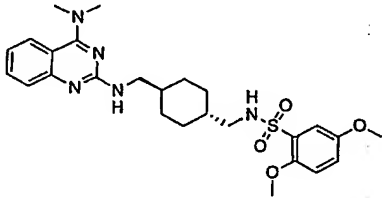
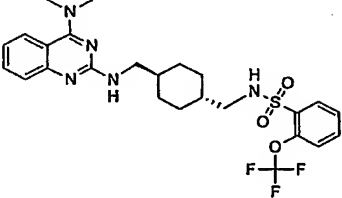
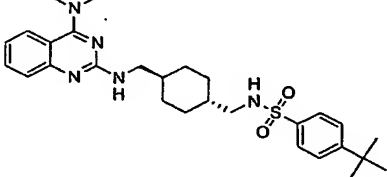
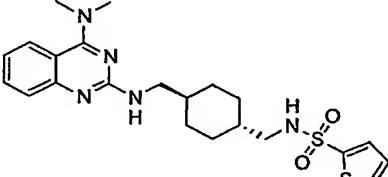
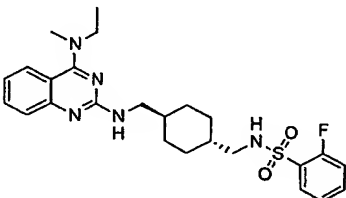
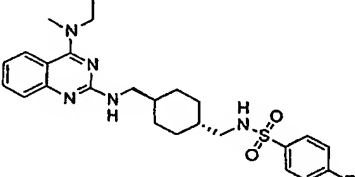
Example No.	Structure	ESI-MS	Retention Time (min)
2573	 $\text{CF}_3\text{CO}_2\text{H}$	570.6 (M + H)	5.23
2574	 $\text{CF}_3\text{CO}_2\text{H}$	805.4 (M + H)	4.91
2575	 $2\text{CF}_3\text{CO}_2\text{H}$	730.8 (M + H)	4.47
2576	 $\text{CF}_3\text{CO}_2\text{H}$	771.6 (M + H)	4.93
2577	 $\text{CF}_3\text{CO}_2\text{H}$	745.6 (M + H)	5.01
2578	 $\text{CF}_3\text{CO}_2\text{H}$	580.8 (M + H)	5.18

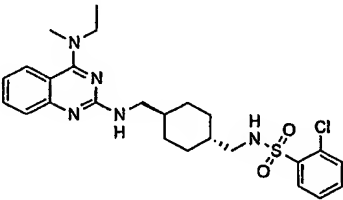
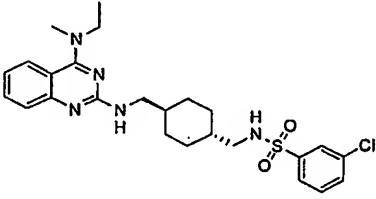
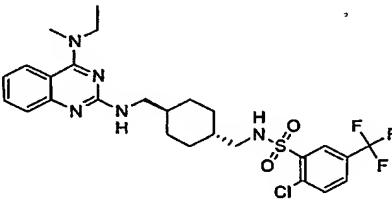
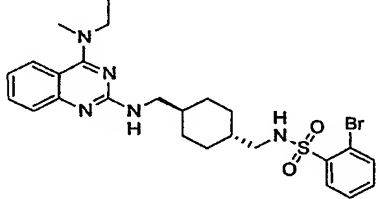
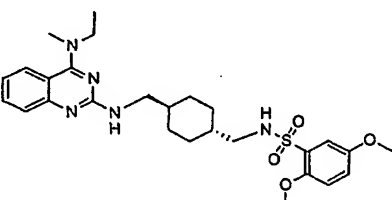
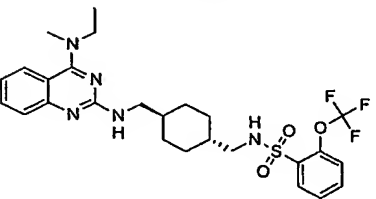
Example No.	Structure	ESI-MS	Retention Time (min)
2579	 2CF ₃ CO ₂ H	621.8 (M + H)	5.27
2580	 CF ₃ CO ₂ H	587.6 (M + H)	4.51
2581	 2CF ₃ CO ₂ H	584.6 (M + H)	4.21
2582	 CF ₃ CO ₂ H	582.8 (M + H)	5.03
2583	 CF ₃ CO ₂ H	653.8 (M + H)	4.90
2584	 CF ₃ CO ₂ H	604.6 (M + H)	5.33

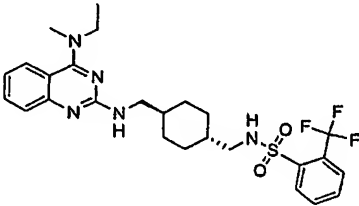
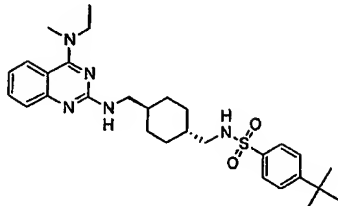
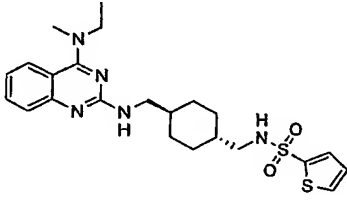
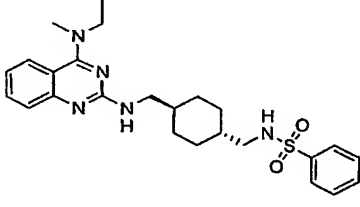
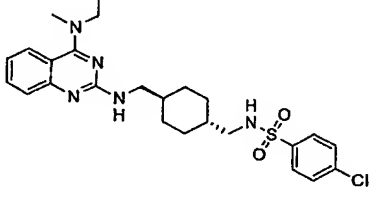
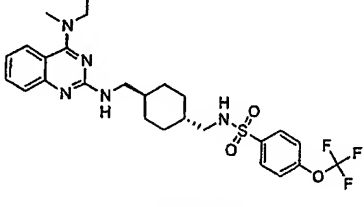
Example No.	Structure	ESI-MS	Retention Time (min)
2585	 <chem>2CF3CO2H</chem>	645.6 (M + H)	5.41
2586	 <chem>CF3CO2H</chem>	458.6 (M + H)	4.39
2587	 <chem>CF3CO2H</chem>	458.6 (M + H)	4.40
2588	 <chem>CF3CO2H</chem>	474.6 (M + H)	4.39
2589	 <chem>CF3CO2H</chem>	474.6 (M + H)	4.58
2590	 <chem>CF3CO2H</chem>	542.6 (M + H)	4.79

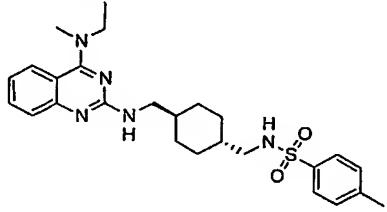
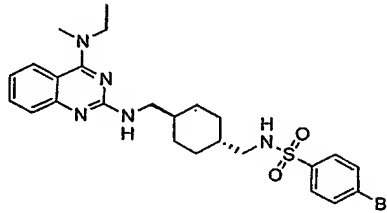
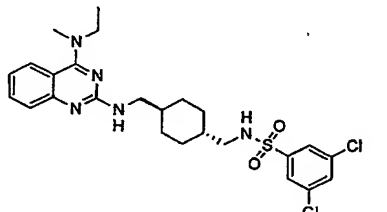
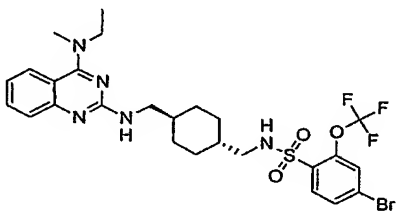
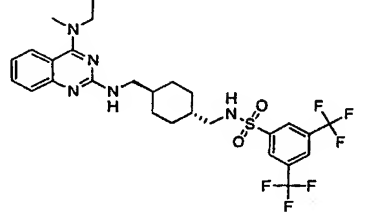
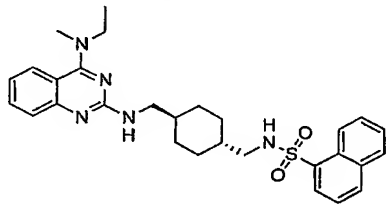
Example No.	Structure	ESI-MS	Retention Time (min)
2591	 <chem>CC1=NC2=C(N1)N=CN=C2CNC3CCCCC3NS(=O)(=O)c4ccccc4Br</chem> $\text{CF}_3\text{CO}_2\text{H}$	518.6 (M + H)	4.51
2592	 <chem>COc1cc(OC)cc(S(=O)(=O)Nc2ccccc2Nc3nc4ccccc4n3)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	500.8 (M + H)	4.33
2593	 <chem>FC(F)(F)c1ccccc1S(=O)(=O)Nc2ccccc2Nc3nc4ccccc4n3</chem> $\text{CF}_3\text{CO}_2\text{H}$	524.6 (M + H)	4.61
2594	 <chem>FC(F)(F)c1ccccc1S(=O)(=O)Nc2ccccc2Nc3nc4ccccc4n3</chem> $\text{CF}_3\text{CO}_2\text{H}$	508.6 (M + H)	4.57
2595	 <chem>CC(C)(C)c1ccc(S(=O)(=O)Nc2ccccc2Nc3nc4ccccc4n3)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	496.8 (M + H)	4.87
2596	 <chem>c1ccsc1S(=O)(=O)Nc2ccccc2Nc3nc4ccccc4n3</chem> $\text{CF}_3\text{CO}_2\text{H}$	446.8 (M + H)	4.29

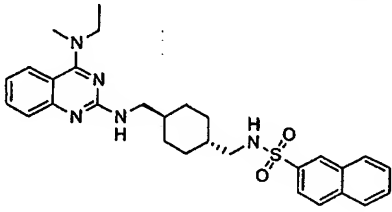
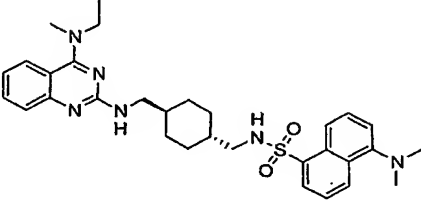
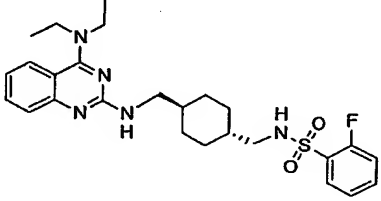
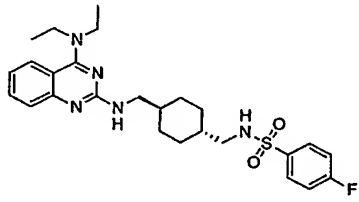
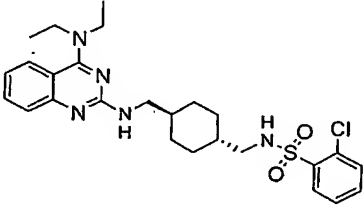
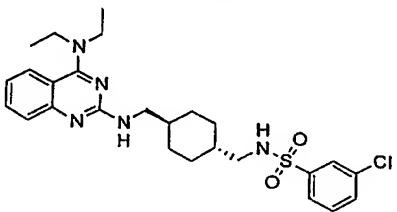
Example No.	Structure	ESI-MS	Retention Time (min)
2597	 <chem>CC1=CN2C(=N1)C=NC2C3CCCCC3CNC(=O)S(=O)(=O)c4ccccc4F</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.8 (M + H)	4.47
2598	 <chem>CC1=CN2C(=N1)C=NC2C3CCCCC3CNC(=O)S(=O)(=O)c4ccc(F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.8 (M + H)	4.53
2599	 <chem>CC1=CN2C(=N1)C=NC2C3CCCCC3CNC(=O)S(=O)(=O)c4ccccc4Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	488.6 (M + H)	4.55
2600	 <chem>CC1=CN2C(=N1)C=NC2C3CCCCC3CNC(=O)S(=O)(=O)c4cccc(Cl)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	487.6 (M + H)	4.65
2601	 <chem>CC1=CN2C(=N1)C=NC2C3CCCCC3CNC(=O)S(=O)(=O)c4cc(C(F)(F)F)ccc4Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	556.6 (M + H)	4.91
2602	 <chem>CC1=CN2C(=N1)C=NC2C3CCCCC3CNC(=O)S(=O)(=O)c4ccccc4Br</chem> $\text{CF}_3\text{CO}_2\text{H}$	532.4 (M + H)	4.61

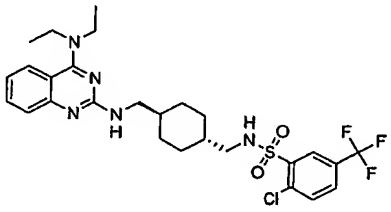
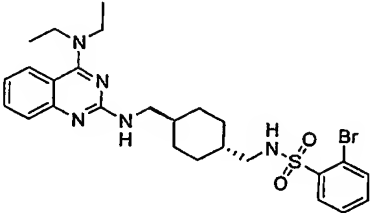
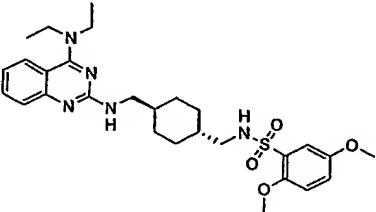
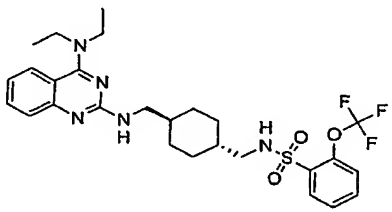
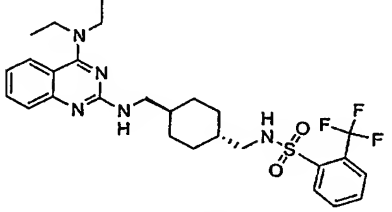
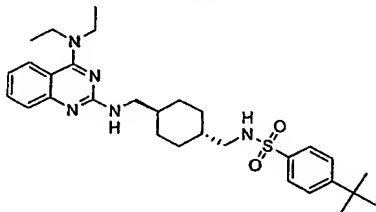
Example No.	Structure	ESI-MS	Retention Time (min)
2603	 <chem>COc1cc(OC)cc(S(=O)(=O)N[C@H]2CCCC[C@H]2CNc3nc4ccccc4n3C)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	514.8 (M + H)	4.43
2604	 <chem>FC(F)(F)c1ccccc1S(=O)(=O)N[C@H]2CCCC[C@H]2CNc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	538.6 (M + H)	4.80
2605	 <chem>CC(C)(C)c1ccc(S(=O)(=O)N[C@H]2CCCC[C@H]2CNc3nc4ccccc4n3C)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	510.6 (M + H)	5.00
2606	 <chem>c1ccsc1S(=O)(=O)N[C@H]2CCCC[C@H]2CNc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	460.6 (M + H)	4.40
2607	 <chem>FC1=CC=C(C=C1)S(=O)(=O)N[C@H]2CCCC[C@H]2CNc3nc4ccccc4n3CN</chem> $\text{CF}_3\text{CO}_2\text{H}$	486.6 (M + H)	4.60
2608	 <chem>FC1=CC=C(C=C1)S(=O)(=O)N[C@H]2CCCC[C@H]2CNc3nc4ccccc4n3CN</chem> $\text{CF}_3\text{CO}_2\text{H}$	484.6 (M + H)	4.64

Example No.	Structure	ESI-MS	Retention Time (min)
2609	 <chem>CCN(C)c1nc2c(ncn2C1CCN(S(=O)(=O)c3cc(Cl)cc3)CC4CCCCC4)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	503.6 (M + H)	4.74
2610	 <chem>CCN(C)c1nc2c(ncn2C1CCN(S(=O)(=O)c3cccc(Cl)c3)CC4CCCCC4)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	502.6 (M + H)	4.86
2611	 <chem>CCN(C)c1nc2c(ncn2C1CCN(S(=O)(=O)c3cc(Cl)cc(C(F)(F)F)c3)CC4CCCCC4)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	570.8 (M + H)	5.00
2612	 <chem>CCN(C)c1nc2c(ncn2C1CCN(S(=O)(=O)c3ccccc3Br)CC4CCCCC4)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	546.0 (M + H)	4.80
2613	 <chem>CCN(C)c1nc2c(ncn2C1CCN(S(=O)(=O)c3cc(OC)cc(OC)c3)CC4CCCCC4)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	528.8 (M + H)	4.63
2614	 <chem>CCN(C)c1nc2c(ncn2C1CCN(S(=O)(=O)c3cc(OC(F)(F)F)ccc3)CC4CCCCC4)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	552.8 (M + H)	4.90

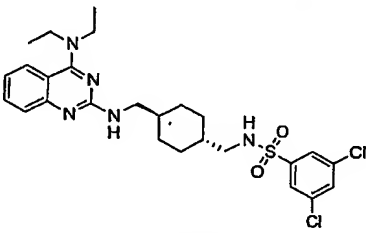
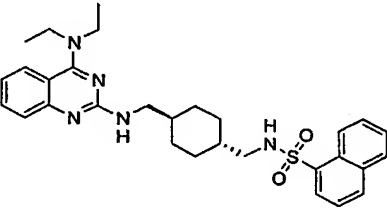
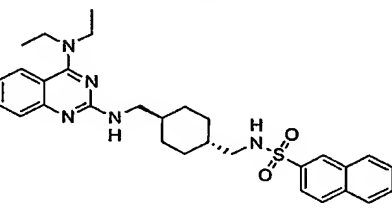
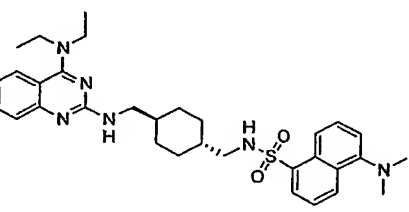
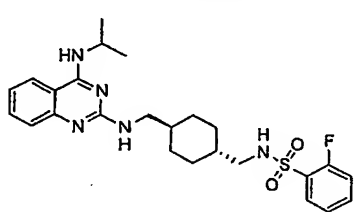
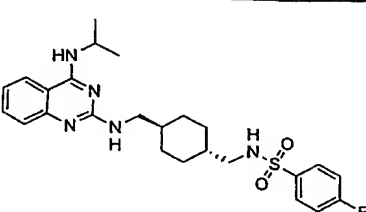
Example No.	Structure	ESI-MS	Retention Time (min)
2615	 <chem>CCN(CC)c1nc2c(ncn2C1CCN3CCCCC3S(=O)(=O)C(F)(F)F)c4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	536.6 (M + H)	4.82
2616	 <chem>CCN(CC)c1nc2c(ncn2C1CCN3CCCCC3S(=O)(=O)c4ccc(C(C)(C)C)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	524.8 (M + H)	5.07
2617	 <chem>CCN(CC)c1nc2c(ncn2C1CCN3CCCCC3S(=O)(=O)c4ccsc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	474.6 (M + H)	4.55
2618	 <chem>CCN(CC)c1nc2c(ncn2C1CCN3CCCCC3S(=O)(=O)c4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	468.4 (M + H)	4.59
2619	 <chem>CCN(CC)c1nc2c(ncn2C1CCN3CCCCC3S(=O)(=O)c4ccc(Cl)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	502.6 (M + H)	4.81
2620	 <chem>CCN(CC)c1nc2c(ncn2C1CCN3CCCCC3S(=O)(=O)c4ccc(OC(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	552.8 (M + H)	4.94

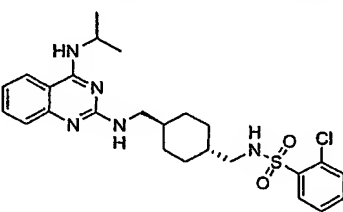
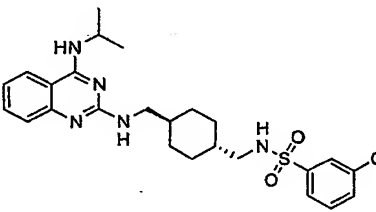
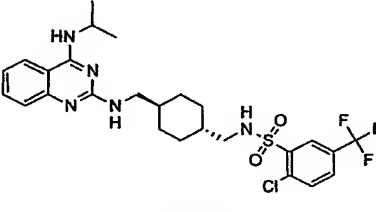
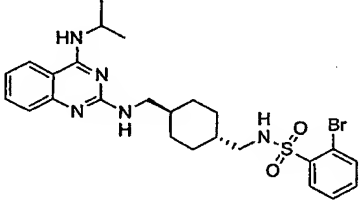
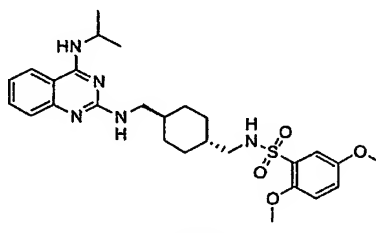
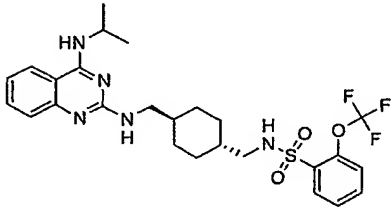
Example No.	Structure	ESI-MS	Retention Time (min)
2621	 <chem>CCN(C)C1=NC2=CC=CC=C2N=C(NC3CCCCC3S(=O)(=O)c4ccc(C)cc4)N1</chem> $\text{CF}_3\text{CO}_2\text{H}$	482.6 (M + H)	4.73
2622	 <chem>CCN(C)C1=NC2=CC=CC=C2N=C(NC3CCCCC3S(=O)(=O)c4ccc(Br)cc4)N1</chem> $\text{CF}_3\text{CO}_2\text{H}$	546.6 (M + H)	4.85
2623	 <chem>CCN(C)C1=NC2=CC=CC=C2N=C(NC3CCCCC3S(=O)(=O)c4cc(Cl)cc(Cl)c4)N1</chem> $\text{CF}_3\text{CO}_2\text{H}$	536.4 (M + H)	5.08
2624	 <chem>CCN(C)C1=NC2=CC=CC=C2N=C(NC3CCCCC3S(=O)(=O)c4cc(OC(F)(F)F)cc(Br)c4)N1</chem> $\text{CF}_3\text{CO}_2\text{H}$	630.4 (M + H)	5.11
2625	 <chem>CCN(C)C1=NC2=CC=CC=C2N=C(NC3CCCCC3S(=O)(=O)c4cc(C(F)(F)F)cc(C(F)(F)F)c4)N1</chem> $\text{CF}_3\text{CO}_2\text{H}$	604.6 (M + H)	5.16
2626	 <chem>CCN(C)C1=NC2=CC=CC=C2N=C(NC3CCCCC3S(=O)(=O)c4c5ccccc5cc4)N1</chem> $\text{CF}_3\text{CO}_2\text{H}$	518.6 (M + H)	4.75

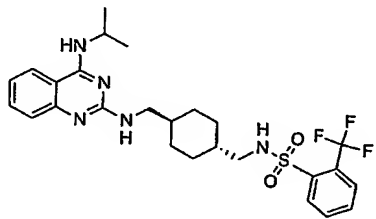
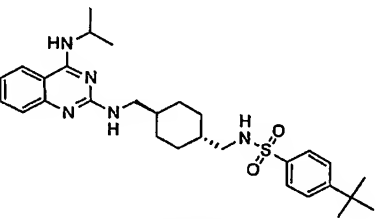
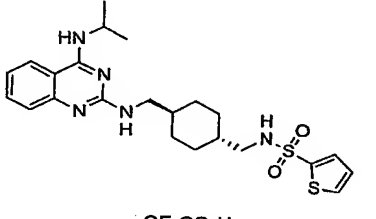
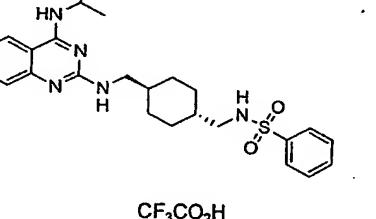
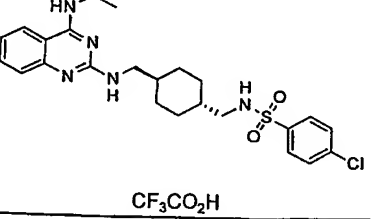
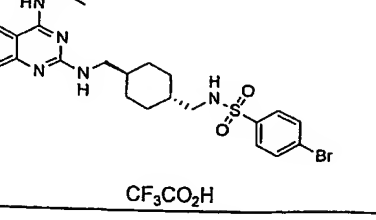
Example No.	Structure	ESI-MS	Retention Time (min)
2627	 $\text{CF}_3\text{CO}_2\text{H}$	518.6 (M + H)	4.91
2628	 $2\text{CF}_3\text{CO}_2\text{H}$	561.6 (M + H)	4.61
2629	 $\text{CF}_3\text{CO}_2\text{H}$	500.8 (M + H)	4.75
2630	 $\text{CF}_3\text{CO}_2\text{H}$	500.2 (M + H)	4.85
2631	 $\text{CF}_3\text{CO}_2\text{H}$	516.6 (M + H)	4.81
2632	 $\text{CF}_3\text{CO}_2\text{H}$	516.6 (M + H)	4.95

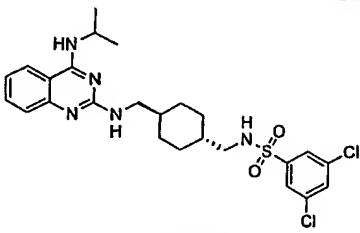
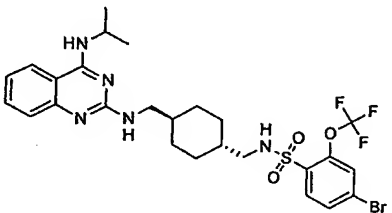
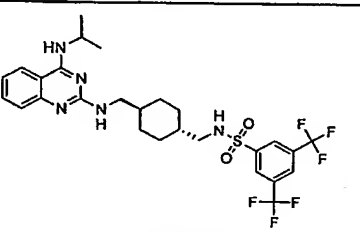
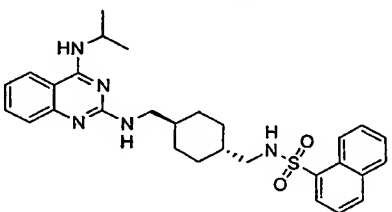
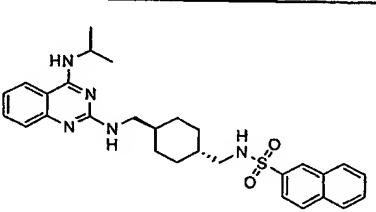
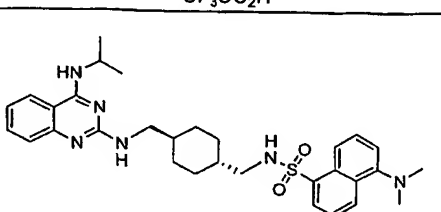
Example No.	Structure	ESI-MS	Retention Time (min)
2633	 <chem>CCN(CC)c1nc2c(ncn2C1CCN(CS(=O)(=O)c3ccc(C(F)(F)F)cc3)CC4CCCCC4)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	584.6 (M + H)	5.18
2634	 <chem>CCN(CC)c1nc2c(ncn2C1CCN(CS(=O)(=O)c3cccc(Br)c3)CC4CCCCC4)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	560.6 (M + H)	4.87
2635	 <chem>CCN(CC)c1nc2c(ncn2C1CCN(CS(=O)(=O)c3cc(OC)cc(OC)c3)CC4CCCCC4)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	542.8 (M + H)	4.80
2636	 <chem>CCN(CC)c1nc2c(ncn2C1CCN(CS(=O)(=O)c3ccccc3OC(F)(F)F)CC4CCCCC4)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	566.6 (M + H)	5.01
2637	 <chem>CCN(CC)c1nc2c(ncn2C1CCN(CS(=O)(=O)c3ccccc3C(F)(F)F)CC4CCCCC4)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	550.8 (M + H)	4.95
2638	 <chem>CCN(CC)c1nc2c(ncn2C1CCN(CS(=O)(=O)c3ccc(C(C)(C)C)cc3)CC4CCCCC4)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	538.6 (M + H)	5.20

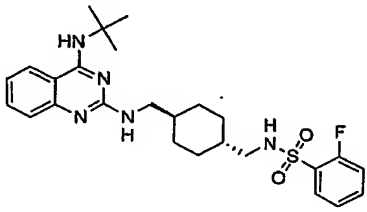
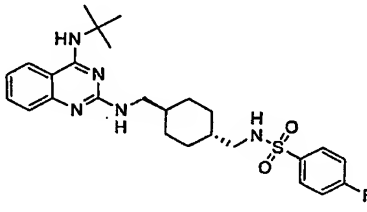
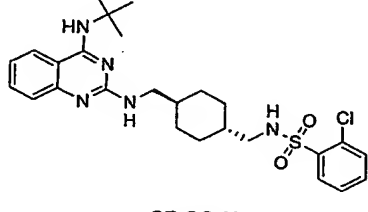
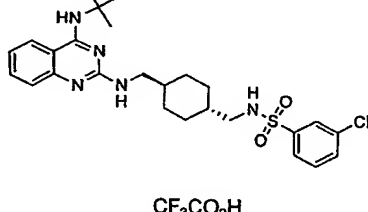
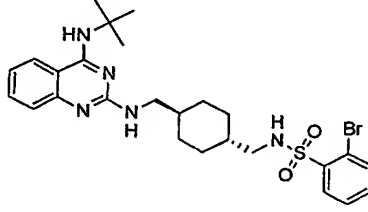
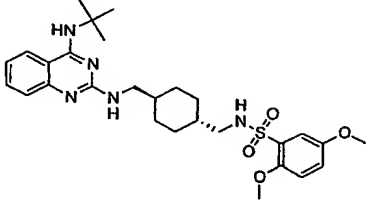
Example No.	Structure	ESI-MS	Retention Time (min)
2639	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4ccc(cc4)S5=CC=CC=C5)C6=CC=CC=C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	488.6 (M + H)	4.65
2640	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4ccccc4)C6=CC=CC=C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	482.6 (M + H)	4.73
2641	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4ccc(cc4)Cl)C6=CC=CC=C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.8 (M + H)	4.97
2642	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4ccc(cc4)OC(F)(F)F)C6=CC=CC=C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	566.6 (M + H)	5.12
2643	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4ccc(cc4)C)C6=CC=CC=C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	496.8 (M + H)	4.89
2644	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4ccc(cc4)Br)C6=CC=CC=C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	560.0 (M + H)	4.98

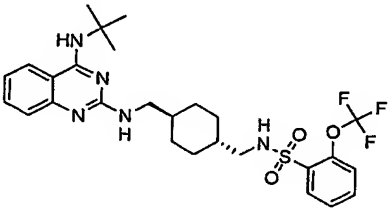
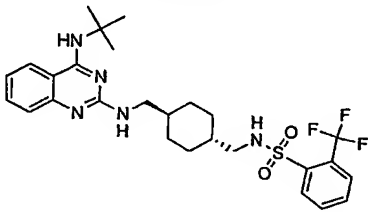
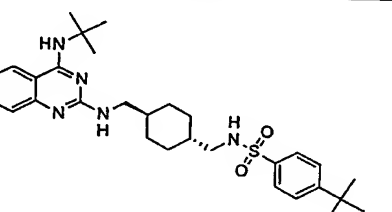
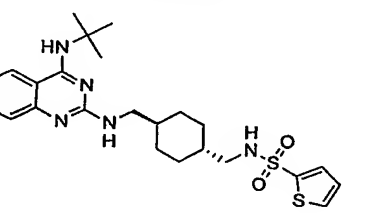
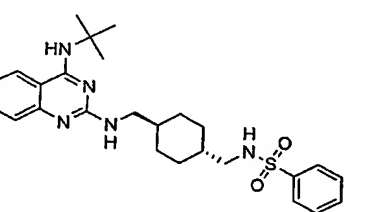
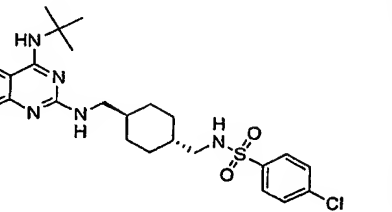
Example No.	Structure	ESI-MS	Retention Time (min)
2645	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4cc(Cl)cc(Cl)c4)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	550.6 (M + H)	5.21
2646	 $\text{CF}_3\text{CO}_2\text{H}$	532.6 (M + H)	4.99
2647	 $\text{CF}_3\text{CO}_2\text{H}$	532.6 (M + H)	5.03
2648	 $2\text{CF}_3\text{CO}_2\text{H}$	575.8 (M + H)	4.80
2649	 $\text{CF}_3\text{CO}_2\text{H}$	486.6 (M + H)	4.64
2650	 $\text{CF}_3\text{CO}_2\text{H}$	486.6 (M + H)	4.66

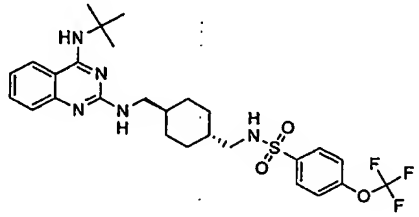
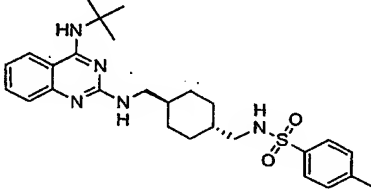
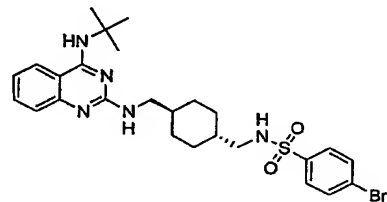
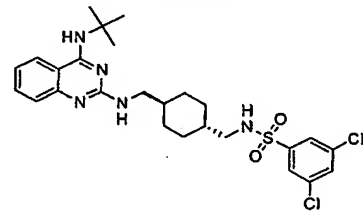
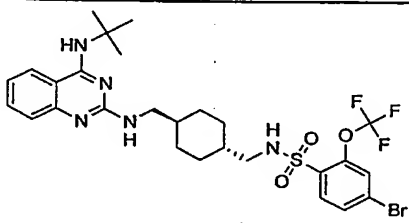
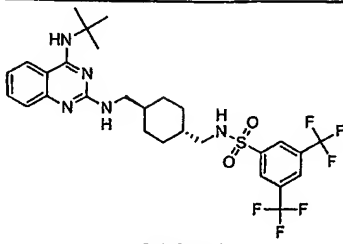
Example No.	Structure	ESI-MS	Retention Time (min)
2651	 <chem>CC(C)Nc1nc2c(ncn2C1CCN1S(=O)(=O)c3ccc(Cl)cc3)c3ccccc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	502.6 (M + H)	4.72
2652	 <chem>CC(C)Nc1nc2c(ncn2C1CCN1S(=O)(=O)c3cccc(Cl)c3)c3ccccc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	502.6 (M + H)	4.87
2653	 <chem>CC(C)Nc1nc2c(ncn2C1CCN1S(=O)(=O)c3cc(C(F)(F)F)cc(Cl)c3)c3ccccc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	570.6 (M + H)	5.03
2654	 <chem>CC(C)Nc1nc2c(ncn2C1CCN1S(=O)(=O)c3cccc(Br)c3)c3ccccc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	546.6 (M + H)	4.77
2655	 <chem>CC(C)Nc1nc2c(ncn2C1CCN1S(=O)(=O)c3cc(OC)cc(OC)c3)c3ccccc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	528.8 (M + H)	4.68
2656	 <chem>CC(C)Nc1nc2c(ncn2C1CCN1S(=O)(=O)c3cc(OC(F)(F)F)ccc3)c3ccccc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	552.8 (M + H)	4.89

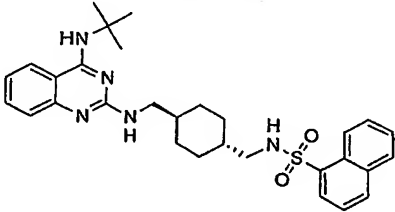
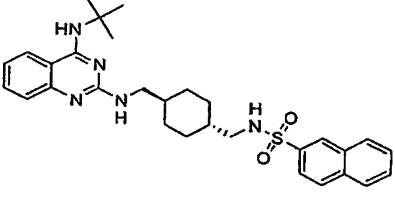
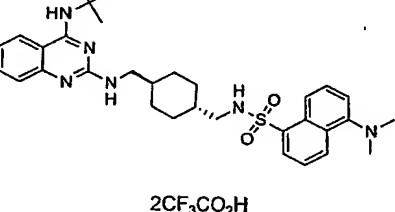
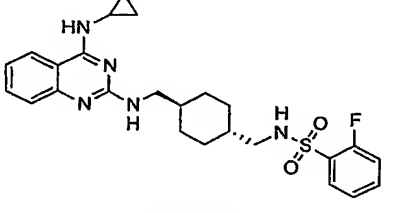
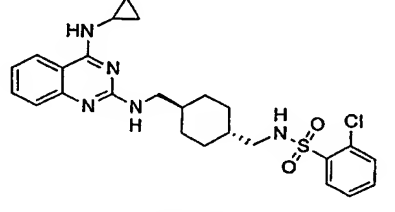
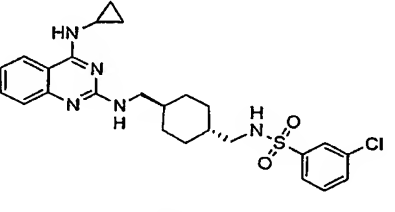
Example No.	Structure	ESI-MS	Retention Time (min)
2657	 <chem>CC(C)Nc1nc2c(ncn2C1CCNCC3CCCCC3NS(=O)(=O)c4ccccc4C(F)(F)F)c3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	536.6 (M + H)	4.85
2658	 <chem>CC(C)Nc1nc2c(ncn2C1CCNCC3CCCCC3NS(=O)(=O)c4ccc(C(C)(C)C)cc4)c3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	524.8 (M + H)	5.15
2659	 <chem>CC(C)Nc1nc2c(ncn2C1CCNCC3CCCCC3NS(=O)(=O)c4ccsc4)c3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	474.8 (M + H)	4.63
2660	 <chem>CC(C)Nc1nc2c(ncn2C1CCNCC3CCCCC3NS(=O)(=O)c4ccccc4)c3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	468.4 (M + H)	4.61
2661	 <chem>CC(C)Nc1nc2c(ncn2C1CCNCC3CCCCC3NS(=O)(=O)c4ccc(Cl)cc4)c3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	502.6 (M + H)	4.86
2662	 <chem>CC(C)Nc1nc2c(ncn2C1CCNCC3CCCCC3NS(=O)(=O)c4ccc(Br)cc4)c3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	546.6 (M + H)	4.64

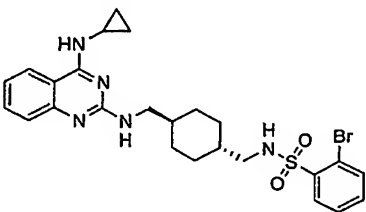
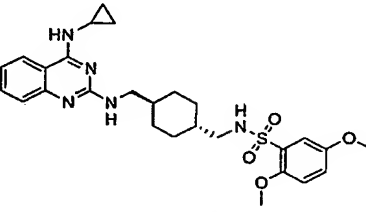
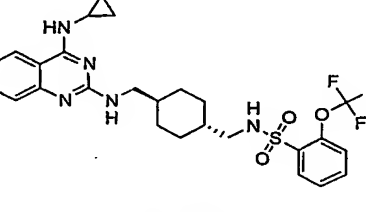
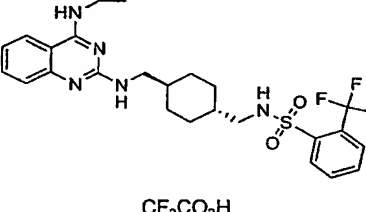
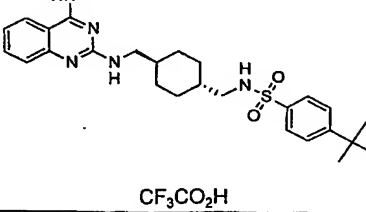
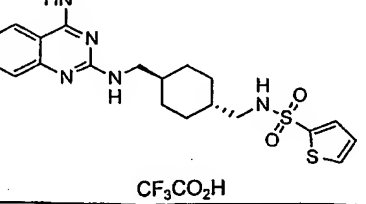
Example No.	Structure	ESI-MS	Retention Time (min)
2663	 $\text{CF}_3\text{CO}_2\text{H}$	536.4 (M + H)	4.81
2664	 $\text{CF}_3\text{CO}_2\text{H}$	630.4 (M + H)	4.85
2665	 $\text{CF}_3\text{CO}_2\text{H}$	604.6 (M + H)	4.87
2666	 $\text{CF}_3\text{CO}_2\text{H}$	518.6 (M + H)	4.67
2667	 $\text{CF}_3\text{CO}_2\text{H}$	518.6 (M + H)	4.90
2668	 $2\text{CF}_3\text{CO}_2\text{H}$	561.6 (M + H)	4.64

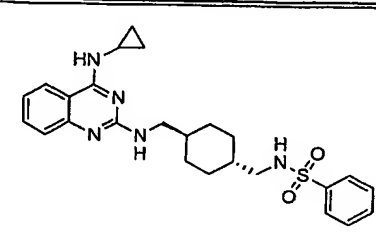
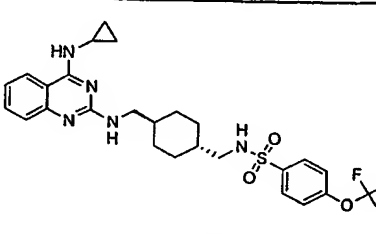
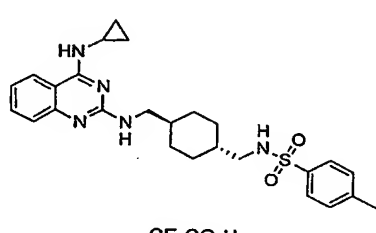
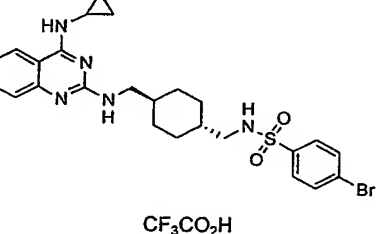
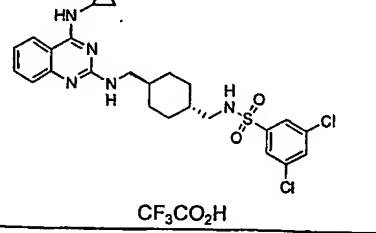
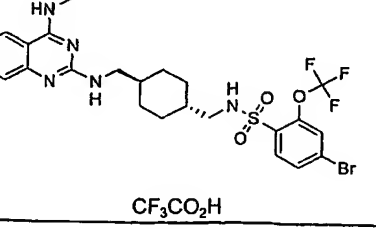
Example No.	Structure	ESI-MS	Retention Time (min)
2669	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCNCCS(=O)(=O)c3cc(F)ccc3)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	500.8 (M + H)	4.73
2670	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCNCCS(=O)(=O)c3ccc(F)cc3)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	500.8 (M + H)	4.74
2671	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCNCCS(=O)(=O)c3ccc(Cl)cc3)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.6 (M + H)	4.89
2672	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCNCCS(=O)(=O)c3cccc(Cl)c3)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.6 (M + H)	4.93
2673	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCNCCS(=O)(=O)c3ccc(Br)cc3)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	560.0 (M + H)	4.89
2674	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCNCCS(=O)(=O)c3cc(OC)cc(OC)c3)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	542.8 (M + H)	4.76

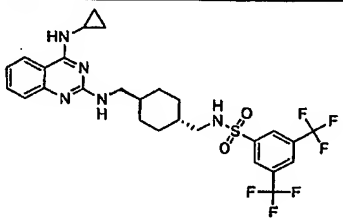
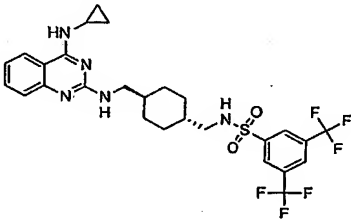
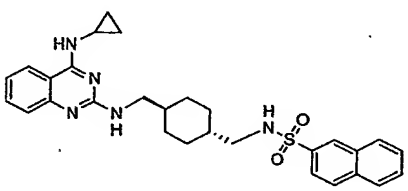
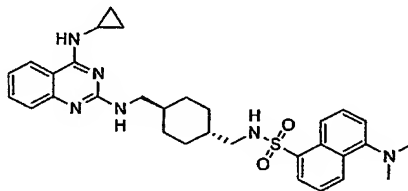
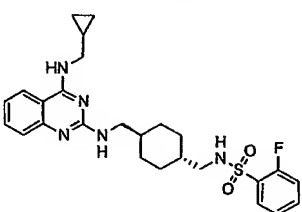
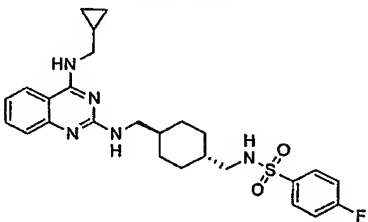
Example No.	Structure	ESI-MS	Retention Time (min)
2675	 <chem>CC(C)(C)Nc1nc2ccccc2n1C3CCCCC3NS(=O)(=O)c4ccccc4C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	566.6 (M + H)	5.03
2676	 <chem>CC(C)(C)Nc1nc2ccccc2n1C3CCCCC3NS(=O)(=O)c4ccccc4C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	550.8 (M + H)	4.96
2677	 <chem>CC(C)(C)Nc1nc2ccccc2n1C3CCCCC3NS(=O)(=O)c4ccc(C(C)(C)C)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	538.8 (M + H)	5.25
2678	 <chem>CC(C)(C)Nc1nc2ccccc2n1C3CCCCC3NS(=O)(=O)c4ccsc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	488.6 (M + H)	4.67
2679	 <chem>CC(C)(C)Nc1nc2ccccc2n1C3CCCCC3NS(=O)(=O)c4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	482.4 (M + H)	4.71
2680	 <chem>CC(C)(C)Nc1nc2ccccc2n1C3CCCCC3NS(=O)(=O)c4ccc(Cl)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.6 (M + H)	4.95

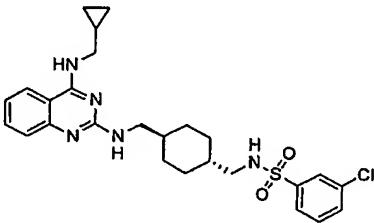
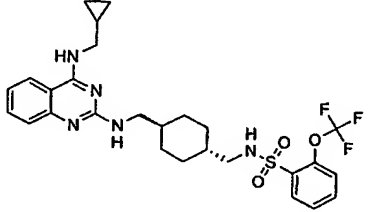
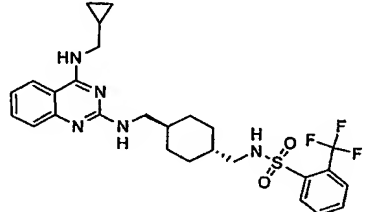
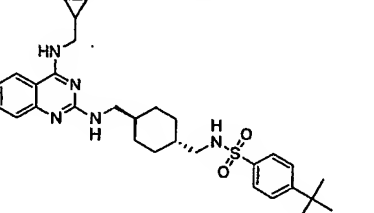
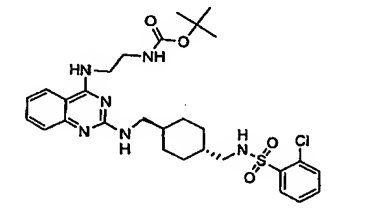
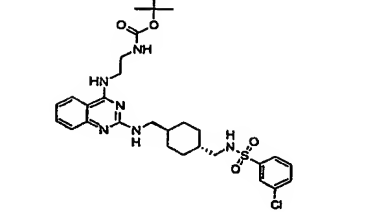
Example No.	Structure	ESI-MS	Retention Time (min)
2681	 <chem>CC(C)(C)N1C=NC2=CC=CC=C2N1CC3CCCCC3NS(=O)(=O)c4ccc(OC(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	566.8 (M + H)	5.07
2682	 <chem>CC(C)(C)N1C=NC2=CC=CC=C2N1CC3CCCCC3NS(=O)(=O)c4ccc(C)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	496.8 (M + H)	4.83
2683	 <chem>CC(C)(C)N1C=NC2=CC=CC=C2N1CC3CCCCC3NS(=O)(=O)c4ccc(Br)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	560.6 (M + H)	5.01
2684	 <chem>CC(C)(C)N1C=NC2=CC=CC=C2N1CC3CCCCC3NS(=O)(=O)c4cc(Cl)cc(Cl)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	550.6 (M + H)	5.07
2685	 <chem>CC(C)(C)N1C=NC2=CC=CC=C2N1CC3CCCCC3NS(=O)(=O)c4cc(Br)cc(OC(F)(F)F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	644.6 (M + H)	5.29
2686	 <chem>CC(C)(C)N1C=NC2=CC=CC=C2N1CC3CCCCC3NS(=O)(=O)c4cc(C(F)(F)F)cc(C(F)(F)F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	618.6 (M + H)	5.25

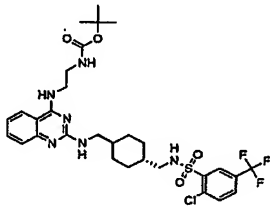
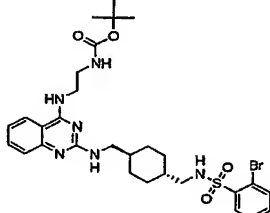
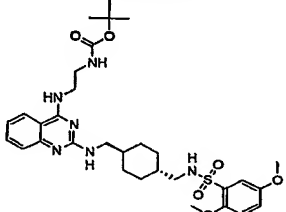
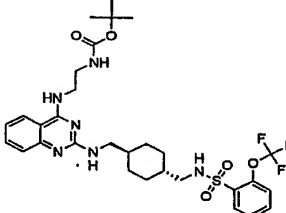
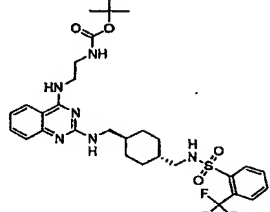
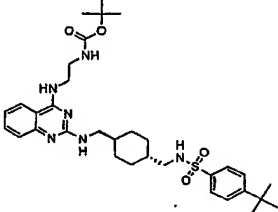
Example No.	Structure	ESI-MS	Retention Time (min)
2687	 <chem>CC(C)(C)Nc1nc2ccccc2n1CN[C@H]3CCCC[C@H]3NS(=O)(=O)c4cccc5ccccc45</chem> $\text{CF}_3\text{CO}_2\text{H}$	532.6 (M + H)	5.01
2688	 <chem>CC(C)(C)Nc1nc2ccccc2n1CN[C@H]3CCCC[C@H]3NS(=O)(=O)c4cccc5ccccc45</chem> $\text{CF}_3\text{CO}_2\text{H}$	532.6 (M + H)	5.04
2689	 <chem>CC(C)(C)Nc1nc2ccccc2n1CN[C@H]3CCCC[C@H]3NS(=O)(=O)c4ccc(C)cc5ccccc45</chem> $2\text{CF}_3\text{CO}_2\text{H}$	575.8 (M + H)	4.75
2690	 <chem>C1CC1Nc2nc3ccccc3n2CN[C@H]4CCCC[C@H]4NS(=O)(=O)c5ccccc5F</chem> $\text{CF}_3\text{CO}_2\text{H}$	484.6 (M + H)	4.51
2691	 <chem>C1CC1Nc2nc3ccccc3n2CN[C@H]4CCCC[C@H]4NS(=O)(=O)c5ccccc5Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	500.8 (M + H)	4.59
2692	 <chem>C1CC1Nc2nc3ccccc3n2CN[C@H]4CCCC[C@H]4NS(=O)(=O)c5ccccc5Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	500.8 (M + H)	4.71

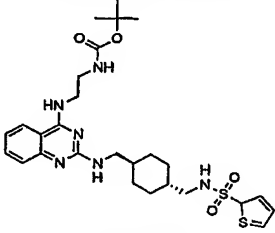
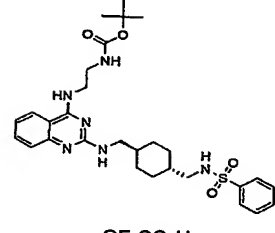
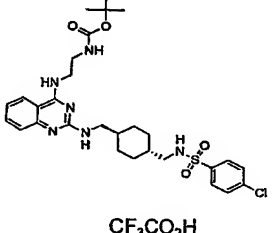
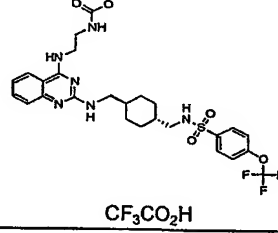
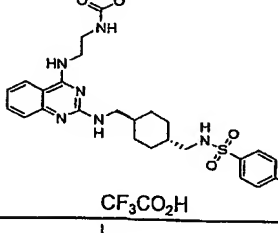
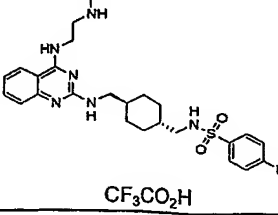
Example No.	Structure	ESI-MS	Retention Time (min)
2693	 <chem>BrC1=CC=C(C=C1)S(=O)(=O)NC2CCCCC2CN3C(=N2)c4ccccc4N3C5CC5</chem> $\text{CF}_3\text{CO}_2\text{H}$	544.6 (M + H)	4.63
2694	 <chem>COc1cc(OC)cc(S(=O)(=O)NC2CCCCC2CN3C(=N2)c4ccccc4N3C5CC5)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	526.8 (M + H)	4.55
2695	 <chem>FC(F)c1cc(S(=O)(=O)NC2CCCCC2CN3C(=N2)c4ccccc4N3C5CC5)ccc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	550.6 (M + H)	4.79
2696	 <chem>FC(F)(F)c1cc(S(=O)(=O)NC2CCCCC2CN3C(=N2)c4ccccc4N3C5CC5)ccc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	534.6 (M + H)	4.69
2697	 <chem>CC(C)(C)c1ccc(S(=O)(=O)NC2CCCCC2CN3C(=N2)c4ccccc4N3C5CC5)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	522.4 (M + H)	5.03
2698	 <chem>c1cc(S(=O)(=O)NC2CCCCC2CN3C(=N2)c4ccccc4N3C5CC5)sc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.8 (M + H)	4.43

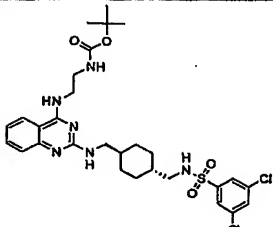
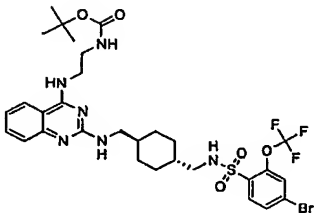
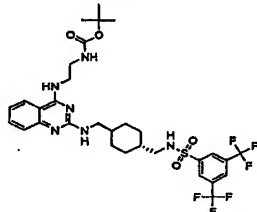
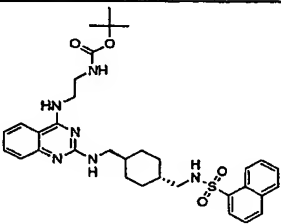
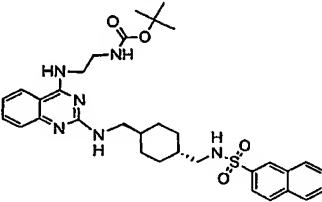
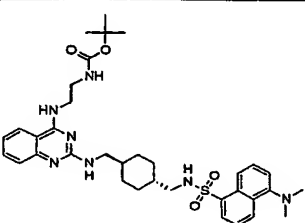
Example No.	Structure	ESI-MS	Retention Time (min)
2699	 <chem>CC1(C)Nc2nc3ccccc3n2NCC4CCCCC4NS(=O)(=O)c5ccccc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	466.6 (M + H)	4.50
2700	 <chem>CC1(C)Nc2nc3ccccc3n2NCC4CCCCC4NS(=O)(=O)c5ccc(OC(F)(F)F)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	550.6 (M + H)	4.87
2701	 <chem>CC1(C)Nc2nc3ccccc3n2NCC4CCCCC4NS(=O)(=O)c5ccc(C)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	480.6 (M + H)	4.65
2702	 <chem>CC1(C)Nc2nc3ccccc3n2NCC4CCCCC4NS(=O)(=O)c5ccc(Br)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	544.6 (M + H)	4.75
2703	 <chem>CC1(C)Nc2nc3ccccc3n2NCC4CCCCC4NS(=O)(=O)c5cc(Cl)cc(Cl)c5</chem> $\text{CF}_3\text{CO}_2\text{H}$	534.6 (M + H)	4.90
2704	 <chem>CC1(C)Nc2nc3ccccc3n2NCC4CCCCC4NS(=O)(=O)c5cc(OC(F)(F)F)cc(Br)c5</chem> $\text{CF}_3\text{CO}_2\text{H}$	628.6 (M + H)	5.08

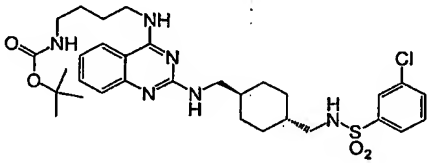
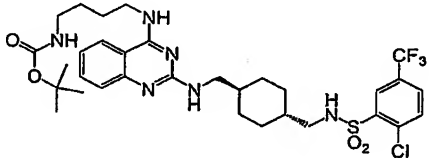
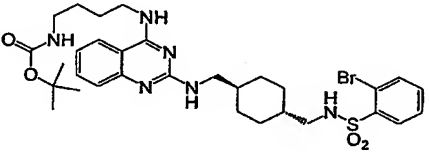
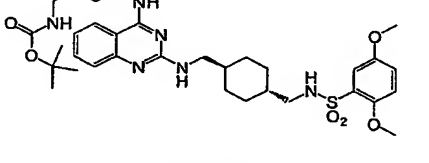
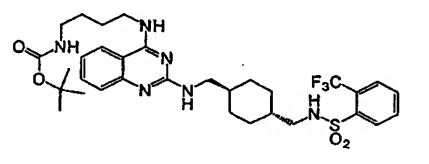
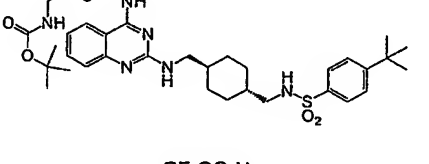
Example No.	Structure	ESI-MS	Retention Time (min)
2705	 <chem>CC1(C)CCCC(C1)NS(=O)(=O)c2ccc(C(F)(F)F)cc2</chem> $\text{CF}_3\text{CO}_2\text{H}$	602.6 (M + H)	5.10
2706	 <chem>CC1(C)CCCC(C1)NS(=O)(=O)c2ccc(C(F)(F)F)cc2</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.8 (M + H)	4.71
2707	 <chem>CC1(C)CCCC(C1)NS(=O)(=O)c2ccc3ccccc3c2</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.8 (M + H)	4.81
2708	 <chem>CC1(C)CCCC(C1)NS(=O)(=O)c2ccc3cc(C)ccc3c2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	559.6 (M + H)	4.50
2709	 <chem>CC1(C)CCCC(C1)NS(=O)(=O)c2cccc(F)c2</chem> $\text{CF}_3\text{CO}_2\text{H}$	498.8 (M + H)	4.64
2710	 <chem>CC1(C)CCCC(C1)NS(=O)(=O)c2ccc(F)cc2</chem> $\text{CF}_3\text{CO}_2\text{H}$	498.8 (M + H)	4.73

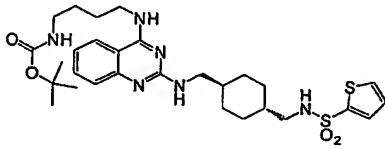
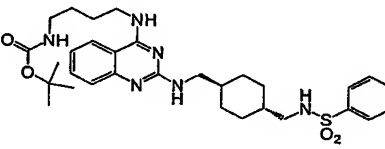
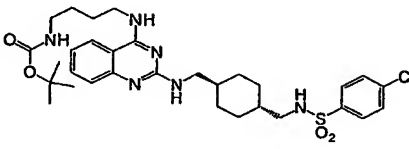
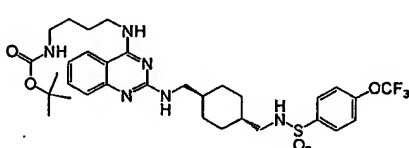
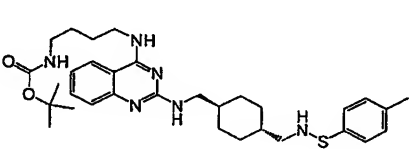
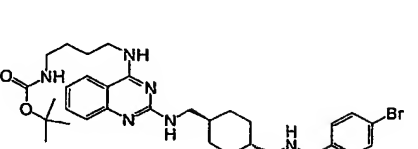
Example No.	Structure	ESI-MS	Retention Time (min)
2711	 <chem>CC1(C)CC1CN2C=NC3C(=N2)N(CS(=O)(=O)c4ccc(Cl)cc4)CC5CCCCC5</chem> $\text{CF}_3\text{CO}_2\text{H}$	514.8 (M + H)	4.87
2712	 <chem>CC1(C)CC1CN2C=NC3C(=N2)N(CS(=O)(=O)c4cc(F)(F)Fcc4)CC5CCCCC5</chem> $\text{CF}_3\text{CO}_2\text{H}$	564.6 (M + H)	4.93
2713	 <chem>CC1(C)CC1CN2C=NC3C(=N2)N(CS(=O)(=O)c4cc(F)(F)Fcc4)CC5CCCCC5</chem> $\text{CF}_3\text{CO}_2\text{H}$	548.6 (M + H)	4.87
2714	 <chem>CC(C)(C)C1=CC=C(C=C1)S(=O)(=O)N(C)CC2CCCCC2N3C=NC4C(=N3)N(CCC5C6C(C)CC6C5)C7=CC=CC=C74</chem> $\text{CF}_3\text{CO}_2\text{H}$	536.6 (M + H)	5.19
2715	 <chem>CC(C)(C)OC(=O)NCCN1C=NC2C(=N1)N(CS(=O)(=O)c3ccc(Cl)cc3)CC4CCCCC4</chem> $\text{CF}_3\text{CO}_2\text{H}$	603.8 (M + H)	4.76
2716	 <chem>CC(C)(C)OC(=O)NCCN1C=NC2C(=N1)N(CS(=O)(=O)c3ccc(Cl)cc3)CC4CCCCC4</chem> $\text{CF}_3\text{CO}_2\text{H}$	603.4 (M + H)	4.87

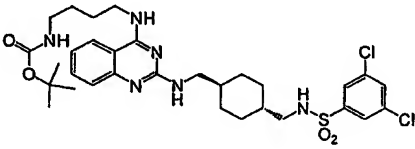
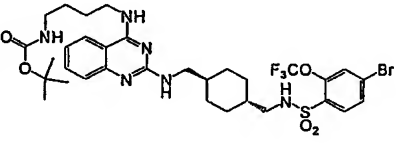
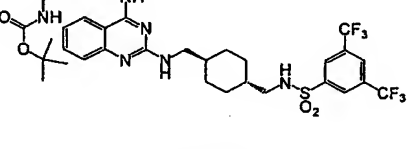
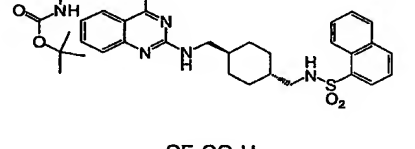
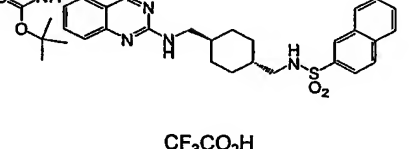
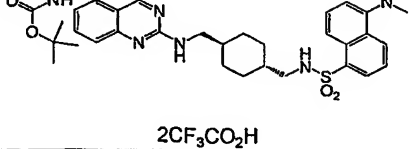
Example No.	Structure	ESI-MS	Retention Time (min)
2717	 $\text{CF}_3\text{CO}_2\text{H}$	671.6 (M + H)	5.05
2718	 $\text{CF}_3\text{CO}_2\text{H}$	647.6 (M + H)	4.79
2719	 $\text{CF}_3\text{CO}_2\text{H}$	629.8 (M + H)	4.67
2720	 $\text{CF}_3\text{CO}_2\text{H}$	653.8 (M + H)	4.91
2721	 $\text{CF}_3\text{CO}_2\text{H}$	637.8 (M + H)	4.85
2722	 $\text{CF}_3\text{CO}_2\text{H}$	625.8 (M + H)	5.14

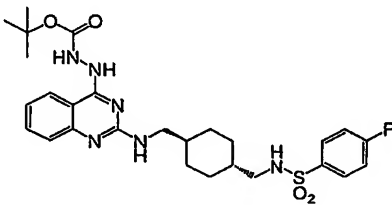
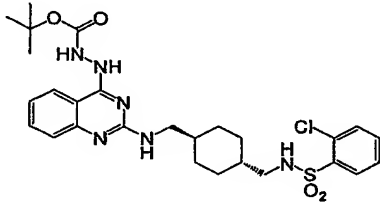
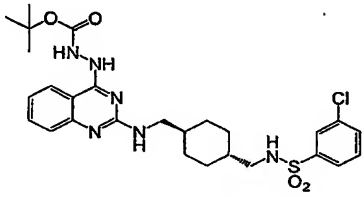
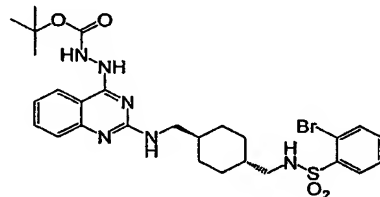
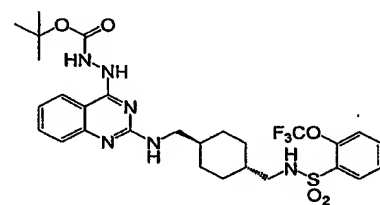
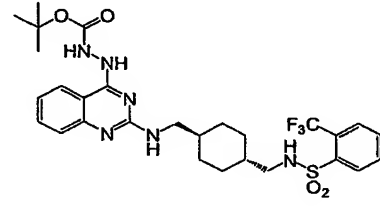
Example No.	Structure	ESI-MS	Retention Time (min)
2723	 <chem>CC(C)(C)OC(=O)NCCNc1nc2c(ncn2C3CCCCC3NS(=O)(=O)c4ccccc4)nc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	575.6 (M + H)	4.63
2724	 <chem>CC(C)(C)OC(=O)NCCNc1nc2c(ncn2C3CCCCC3NS(=O)(=O)c4ccccc4)nc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	569.8 (M + H)	4.66
2725	 <chem>CC(C)(C)OC(=O)NCCNc1nc2c(ncn2C3CCCCC3NS(=O)(=O)c4ccc(Cl)cc4)nc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	603.8 (M + H)	4.88
2726	 <chem>CC(C)(C)OC(=O)NCCNc1nc2c(ncn2C3CCCCC3NS(=O)(=O)c4ccc(OC(F)(F)F)cc4)nc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	653.8 (M + H)	5.01
2727	 <chem>CC(C)(C)OC(=O)NCCNc1nc2c(ncn2C3CCCCC3NS(=O)(=O)c4ccccc4)nc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	583.8 (M + H)	4.77
2728	 <chem>CC(C)(C)OC(=O)NCCNc1nc2c(ncn2C3CCCCC3NS(=O)(=O)c4ccc(Br)cc4)nc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	647 (M + H)	4.92

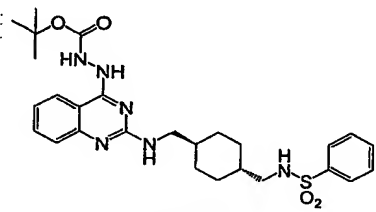
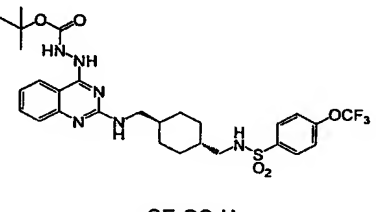
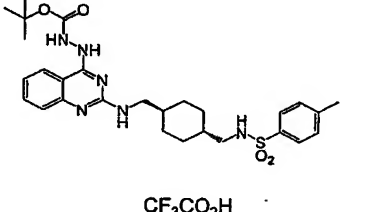
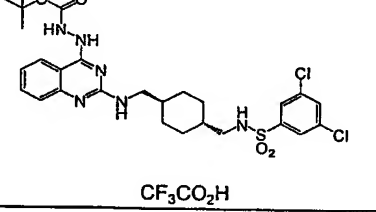
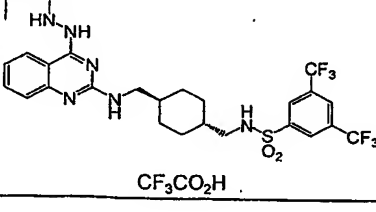
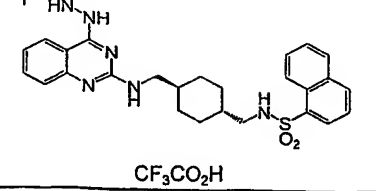
Example No.	Structure	ESI-MS	Retention Time (min)
2729	 $\text{CF}_3\text{CO}_2\text{H}$	637.8 (M + H)	5.13
2730	 $\text{CF}_3\text{CO}_2\text{H}$	731.6 (M + H)	5.19
2731	 $\text{CF}_3\text{CO}_2\text{H}$	705.8 (M + H)	5.22
2732	 $\text{CF}_3\text{CO}_2\text{H}$	619.8 (M + H)	4.91
2733	 $\text{CF}_3\text{CO}_2\text{H}$	619.8 (M + H)	4.93
2734	 $2\text{CF}_3\text{CO}_2\text{H}$	663.0 (M + H)	4.67

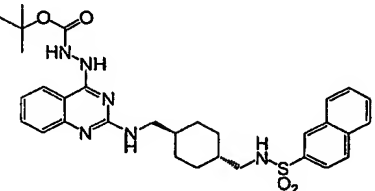
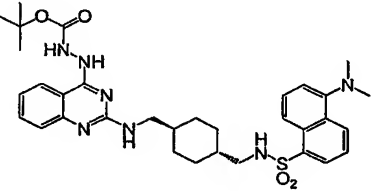
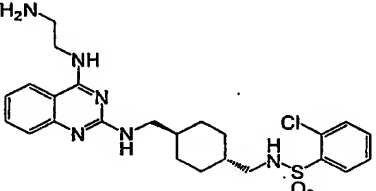
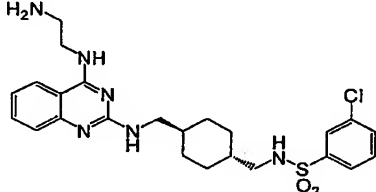
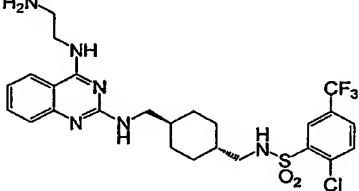
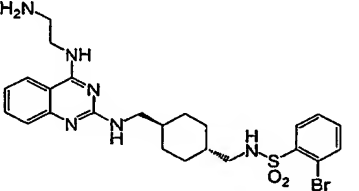
Example No.	Structure	ESI-MS	Retention Time (min)
2735	 $\text{CF}_3\text{CO}_2\text{H}$	631.8 (M + H)	5.01
2736	 $\text{CF}_3\text{CO}_2\text{H}$	699.0 (M + H)	5.19
2737	 $\text{CF}_3\text{CO}_2\text{H}$	675.8 (M + H)	4.95
2738	 $\text{CF}_3\text{CO}_2\text{H}$	657.8 (M + H)	4.81
2739	 $\text{CF}_3\text{CO}_2\text{H}$	665.8 (M + H)	4.97
2740	 $\text{CF}_3\text{CO}_2\text{H}$	653.8 (M + H)	5.27

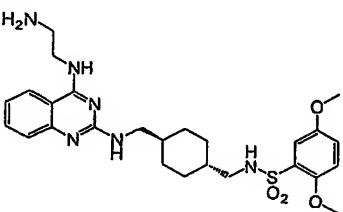
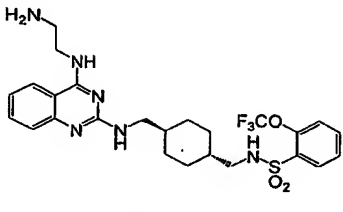
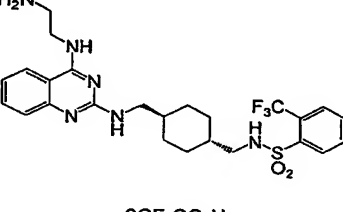
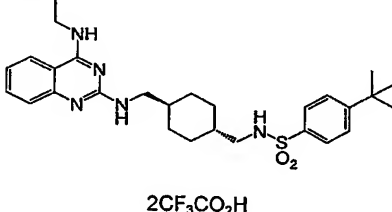
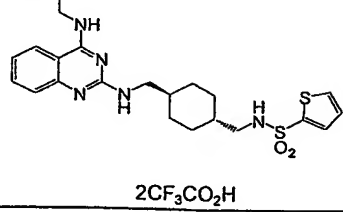
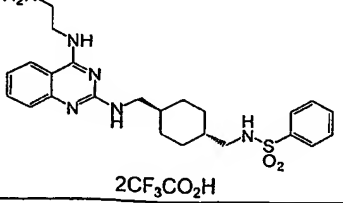
Example No.	Structure	ESI-MS	Retention Time (min)
2741	 $\text{CF}_3\text{CO}_2\text{H}$	603.4 (M + H)	4.77
2742	 $\text{CF}_3\text{CO}_2\text{H}$	597.8 (M + H)	4.79
2743	 $\text{CF}_3\text{CO}_2\text{H}$	631.8 (M + H)	5.02
2744	 $\text{CF}_3\text{CO}_2\text{H}$	681.8 (M + H)	5.14
2745	 $\text{CF}_3\text{CO}_2\text{H}$	611.8 (M + H)	4.93
2746	 $\text{CF}_3\text{CO}_2\text{H}$	675.0 (M + H)	5.05

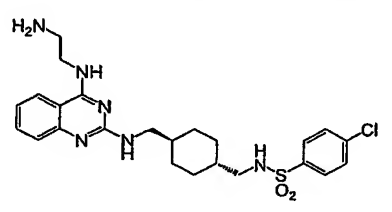
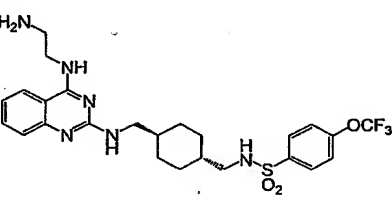
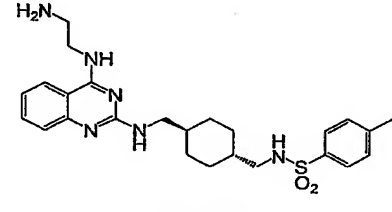
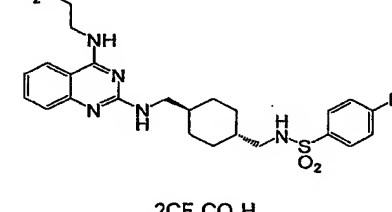
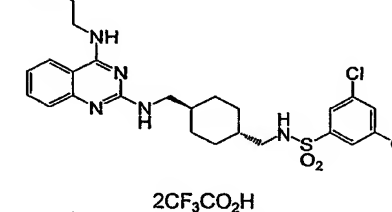
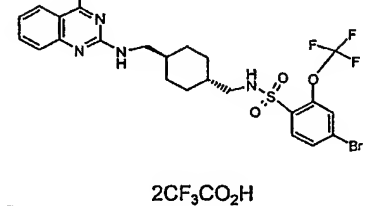
Example No.	Structure	ESI-MS	Retention Time (min)
2747	 $\text{CF}_3\text{CO}_2\text{H}$	665.8 (M + H)	5.29
2748	 $\text{CF}_3\text{CO}_2\text{H}$	759.6 (M + H)	5.31
2749	 $\text{CF}_3\text{CO}_2\text{H}$	733.8 (M + H)	5.36
2750	 $\text{CF}_3\text{CO}_2\text{H}$	647.8 (M + H)	5.05
2751	 $\text{CF}_3\text{CO}_2\text{H}$	647.8 (M + H)	5.08
2752	 $2\text{CF}_3\text{CO}_2\text{H}$	691.0 (M + H)	4.89

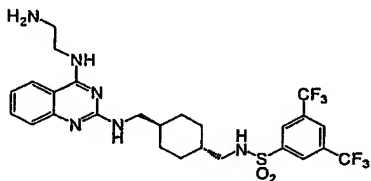
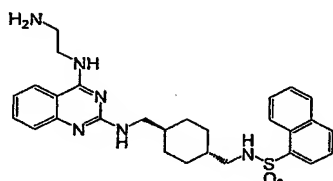
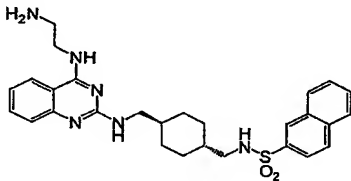
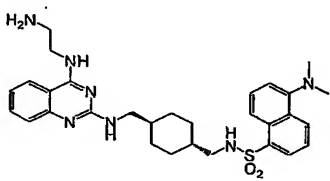
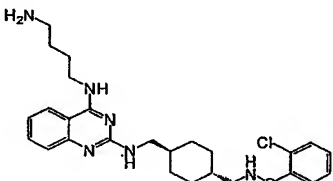
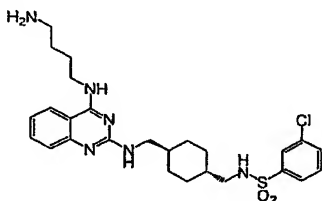
Example No.	Structure	ESI-MS	Retention Time (min)
2753	 <chem>CC(C)(C)OC(=O)NNc1nc2ccccc2n1CNC3CCCCC3CNS(=O)(=O)c4ccc(F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	559.6 (M + H)	4.51
2754	 <chem>CC(C)(C)OC(=O)NNc1nc2ccccc2n1CNC3CCCCC3CNS(=O)(=O)c4ccc(Cl)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	575.6 (M + H)	4.57
2755	 <chem>CC(C)(C)OC(=O)NNc1nc2ccccc2n1CNC3CCCCC3CNS(=O)(=O)c4cc(Cl)ccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	575.6 (M + H)	4.69
2756	 <chem>CC(C)(C)OC(=O)NNc1nc2ccccc2n1CNC3CCCCC3CNS(=O)(=O)c4ccc(Br)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	619.6 (M + H)	4.63
2757	 <chem>CC(C)(C)OC(=O)NNc1nc2ccccc2n1CNC3CCCCC3CNS(=O)(=O)c4ccc(OC(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	625.8 (M + H)	4.72
2758	 <chem>CC(C)(C)OC(=O)NNc1nc2ccccc2n1CNC3CCCCC3CNS(=O)(=O)c4ccc(C(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	609.8 (M + H)	4.67

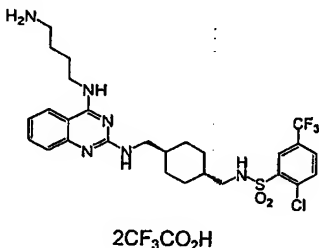
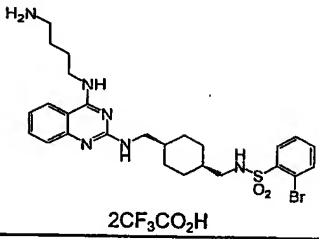
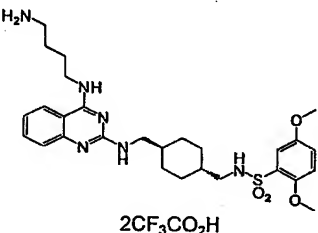
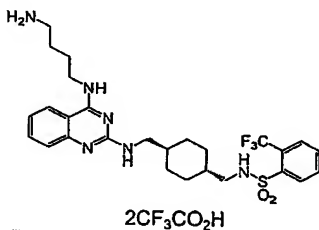
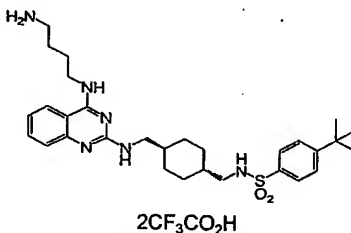
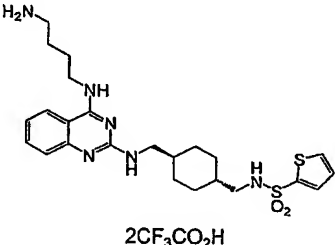
Example No.	Structure	ESI-MS	Retention Time (min)
2759	 <chem>CC(C)(C)OC(=O)NNc1nc2ccccc2n1CNCC3CCCCC3NS(=O)(=O)c4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	541.8 (M + H)	4.45
2760	 <chem>CC(C)(C)OC(=O)NNc1nc2ccccc2n1CNCC3CCCCC3NS(=O)(=O)c4ccc(OC(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	625.8 (M + H)	4.38
2761	 <chem>CC(C)(C)OC(=O)NNc1nc2ccccc2n1CNCC3CCCCC3NS(=O)(=O)c4ccc(C)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	555.8 (M + H)	4.57
2762	 <chem>CC(C)(C)OC(=O)NNc1nc2ccccc2n1CNCC3CCCCC3NS(=O)(=O)c4cc(Cl)cc(Cl)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	609.8 (M + H)	4.94
2763	 <chem>CC(C)(C)OC(=O)NNc1nc2ccccc2n1CNCC3CCCCC3NS(=O)(=O)c4cc(C(F)(F)F)cc(C(F)(F)F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	677.8 (M + H)	5.05
2764	 <chem>CC(C)(C)OC(=O)NNc1nc2ccccc2n1CNCC3CCCCC3NS(=O)(=O)c4c5ccccc5cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	591.6 (M + H)	4.73

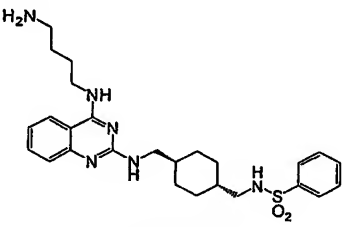
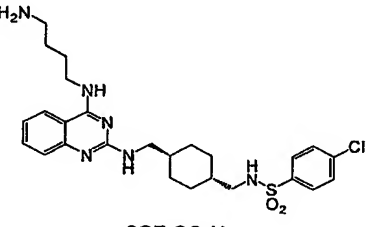
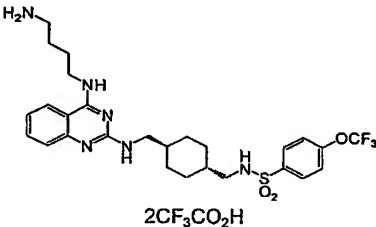
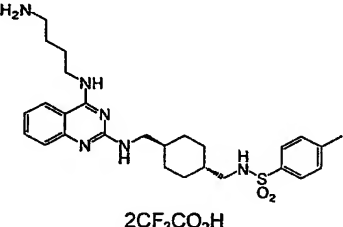
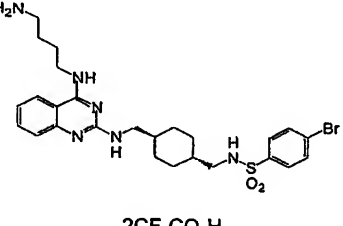
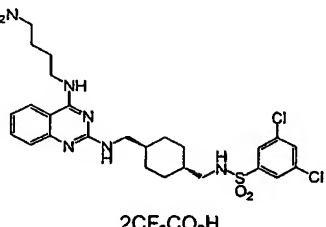
Example No.	Structure	ESI-MS	Retention Time (min)
2765	 $\text{CF}_3\text{CO}_2\text{H}$	591.6 (M + H)	4.75
2766	 $2\text{CF}_3\text{CO}_2\text{H}$	635.0 (M + H)	4.47
2767	 $2\text{CF}_3\text{CO}_2\text{H}$	503.6 (M + H)	3.83
2768	 $2\text{CF}_3\text{CO}_2\text{H}$	503.6 (M + H)	3.99
2769	 $2\text{CF}_3\text{CO}_2\text{H}$	571.6 (M + H)	4.16
2770	 $2\text{CF}_3\text{CO}_2\text{H}$	547.6 (M + H)	3.85

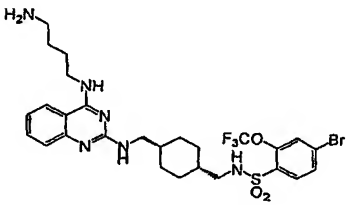
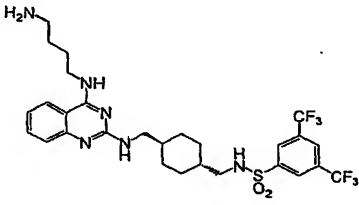
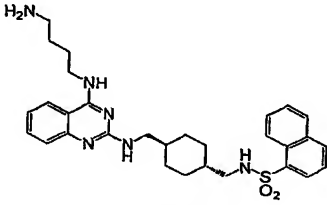
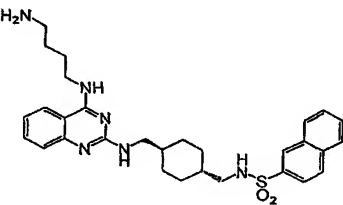
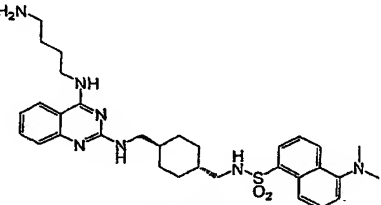
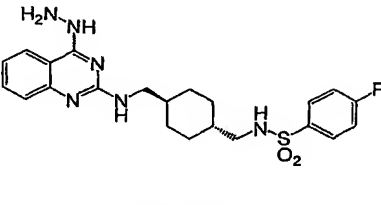
Example No.	Structure	ESI-MS	Retention Time (min)
2771	 <chem>2CF3CO2H</chem>	529.6 (M + H)	3.75
2772	 <chem>2CF3CO2H</chem>	553.8 (M + H)	3.99
2773	 <chem>2CF3CO2H</chem>	537.6 (M + H)	3.93
2774	 <chem>2CF3CO2H</chem>	525.8 (M + H)	4.22
2775	 <chem>2CF3CO2H</chem>	475.6 (M + H)	3.64
2776	 <chem>2CF3CO2H</chem>	469.6 (M + H)	3.71

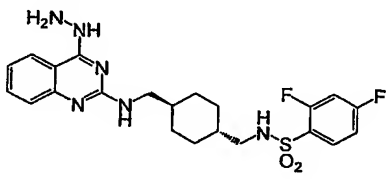
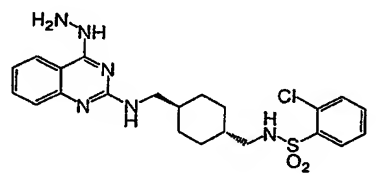
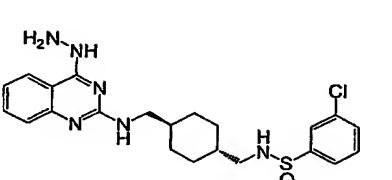
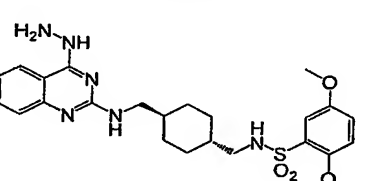
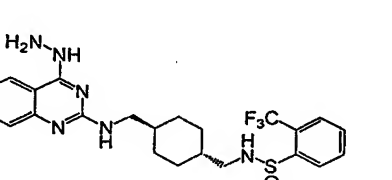
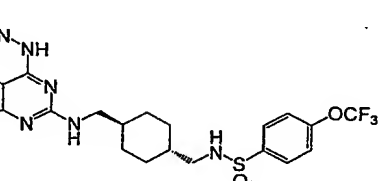
Example No.	Structure	ESI-MS	Retention Time (min)
2777	 <chem>NCCNC1=NC2=CC=CC=C2N=C(NC1CC3CCCCC3CNS(=O)(=O)C4=CC=C(Cl)C=C4)N3</chem> $2CF_3CO_2H$	503.6 (M + H)	3.97
2778	 <chem>NCCNC1=NC2=CC=CC=C2N=C(NC1CC3CCCCC3CNS(=O)(=O)C4=CC=C(OC(F)(F)F)C=C4)N3</chem> $2CF_3CO_2H$	553.8 (M + H)	4.17
2779	 <chem>NCCNC1=NC2=CC=CC=C2N=C(NC1CC3CCCCC3CNS(=O)(=O)C4=CC=C(C)C=C4)N3</chem> $2CF_3CO_2H$	483.4 (M + H)	3.87
2780	 <chem>NCCNC1=NC2=CC=CC=C2N=C(NC1CC3CCCCC3CNS(=O)(=O)C4=CC=C(Br)C=C4)N3</chem> $2CF_3CO_2H$	547.6 (M + H)	4.04
2781	 <chem>NCCNC1=NC2=CC=CC=C2N=C(NC1CC3CCCCC3CNS(=O)(=O)C4=CC(=C(Cl)C=C(Cl))C=C4)N3</chem> $2CF_3CO_2H$	537.4 (M + H)	4.23
2782	 <chem>NCCNC1=NC2=CC=CC=C2N=C(NC1CC3CCCCC3CNS(=O)(=O)C4=CC(=C(Br)C=C(OC(F)(F)F))C=C4)N3</chem> $2CF_3CO_2H$	631.6 (M + H)	4.23

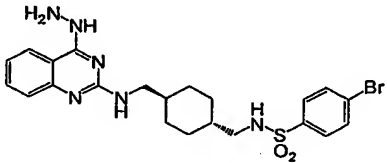
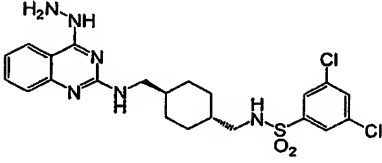
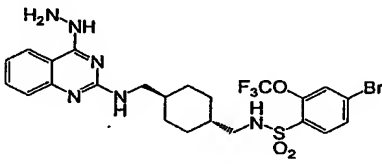
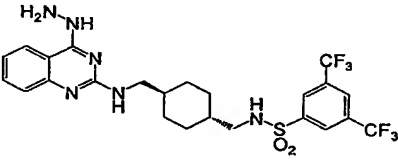
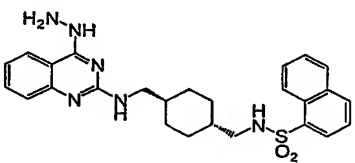
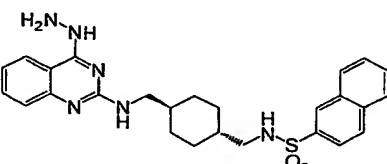
Example No.	Structure	ESI-MS	Retention Time (min)
2783	 $2\text{CF}_3\text{CO}_2\text{H}$	605.8 (M + H)	4.41
2784	 $2\text{CF}_3\text{CO}_2\text{H}$	519.6 (M + H)	4.01
2785	 $2\text{CF}_3\text{CO}_2\text{H}$	519.6 (M + H)	4.07
2786	 $3\text{CF}_3\text{CO}_2\text{H}$	562.6 (M + H)	3.77
2787	 $2\text{CF}_3\text{CO}_2\text{H}$	531.6 (M + H)	3.90
2788	 $2\text{CF}_3\text{CO}_2\text{H}$	531.6 (M + H)	4.04

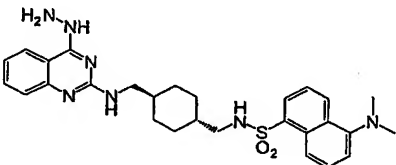
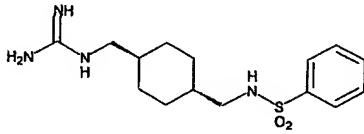
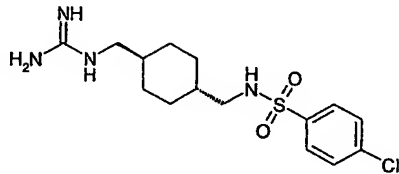
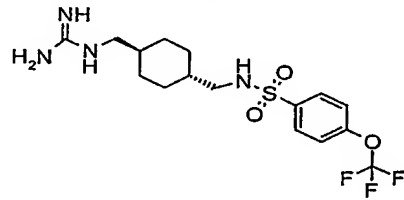
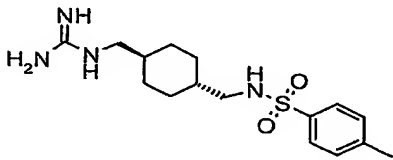
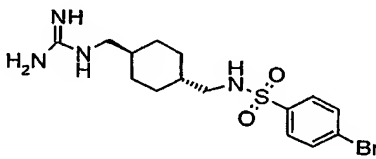
Example No.	Structure	ESI-MS	Retention Time (min)
2789	 <chem>2CF3CO2H</chem>	599.6 (M + H)	4.24
2790	 <chem>2CF3CO2H</chem>	575.0 (M + H)	3.95
2791	 <chem>2CF3CO2H</chem>	557.6 (M + H)	3.86
2792	 <chem>2CF3CO2H</chem>	565.6 (M + H)	4.03
2793	 <chem>2CF3CO2H</chem>	554 (M + H)	4.29
2794	 <chem>2CF3CO2H</chem>	503.6 (M + H)	3.78

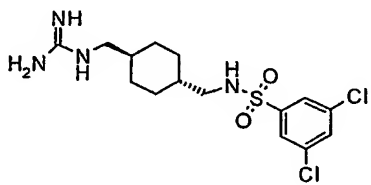
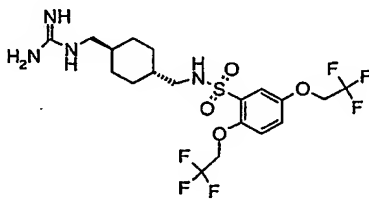
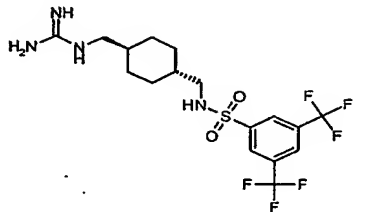
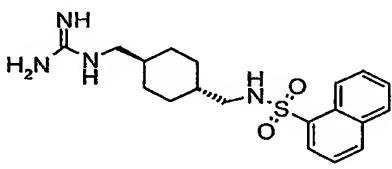
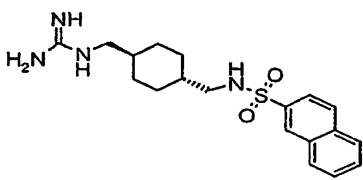
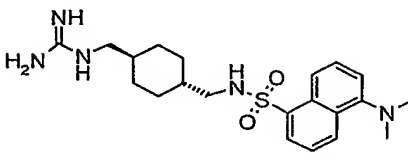
Example No.	Structure	ESI-MS	Retention Time (min)
2795	 2CF ₃ CO ₂ H	497.6 (M + H)	3.83
2796	 2CF ₃ CO ₂ H	531.6 (M + H)	4.05
2797	 2CF ₃ CO ₂ H	582.0 (M + H)	4.23
2798	 2CF ₃ CO ₂ H	511 (M + H)	3.95
2799	 2CF ₃ CO ₂ H	575.6 (M + H)	4.10
2800	 2CF ₃ CO ₂ H	565.0 (M + H)	4.32

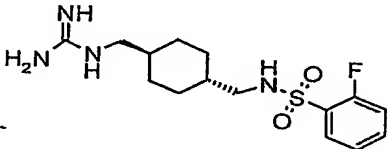
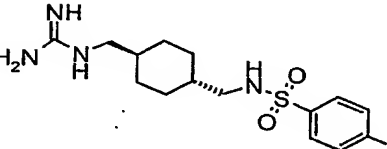
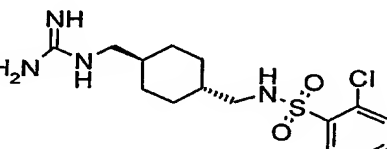
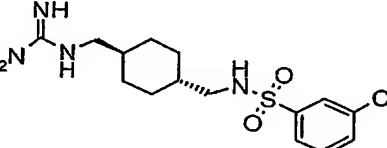
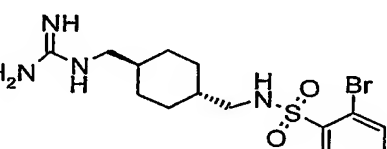
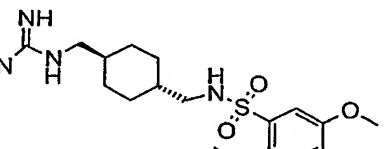
Example No.	Structure	ESI-MS	Retention Time (min)
2801	 2CF ₃ CO ₂ H	659.6 (M + H)	4.35
2802	 2CF ₃ CO ₂ H	634.0 (M + H)	4.43
2803	 2CF ₃ CO ₂ H	547.6 (M + H)	4.09
2804	 2CF ₃ CO ₂ H	547.6 (M + H)	4.15
2805	 3CF ₃ CO ₂ H	590.6 (M + H)	3.93
2806	 2CF ₃ CO ₂ H	459.6 (M + H)	4.07

Example No.	Structure	ESI-MS	Retention Time (min)
2807	 <chem>Nc1nc2c(ncn2C1CCN3CCSC(=O)c4cc(F)cc(F)c4)CC3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	477.6 (M + H)	4.07
2808	 <chem>Nc1nc2c(ncn2C1CCN3CCSC(=O)c4ccccc4Cl)CC3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	475.6 (M + H)	4.07
2809	 <chem>Nc1nc2c(ncn2C1CCN3CCSC(=O)c4ccc(Cl)cc4)CC3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	475.6 (M + H)	4.23
2810	 <chem>Nc1nc2c(ncn2C1CCN3CCSC(=O)c4cc(OC)cc(OC)c4)CC3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	501.8 (M + H)	4.15
2811	 <chem>Nc1nc2c(ncn2C1CCN3CCSC(=O)c4ccccc4C(F)(F)F)CC3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	509.4 (M + H)	4.27
2812	 <chem>Nc1nc2c(ncn2C1CCN3CCSC(=O)c4ccc(OC(F)(F)F)cc4)CC3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	525.6 (M + H)	4.37

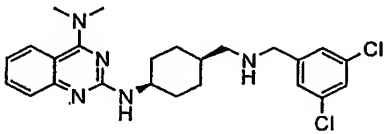
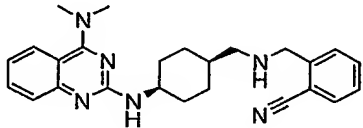
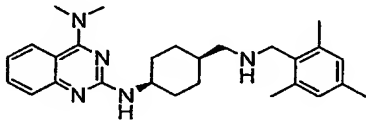
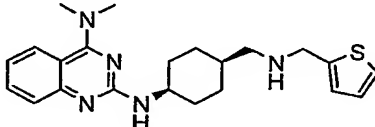
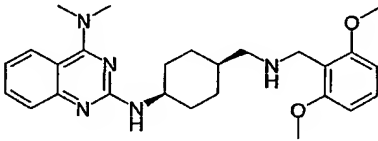
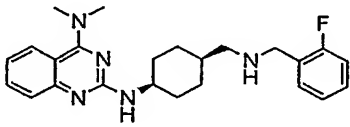
Example No.	Structure	ESI-MS	Retention Time (min)
2813	 <chem>Nc1nc2ccccc2n1C3CCCCC3C4=CC=C(C=C4)S(=O)(=O)c5ccc(Br)cc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	519.6 (M + H)	4.25
2814	 <chem>Nc1nc2ccccc2n1C3CCCCC3C4=CC=C(C=C4)S(=O)(=O)c5cc(Cl)cc(Cl)c5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	509.4 (M + H)	4.49
2815	 <chem>Nc1nc2ccccc2n1C3CCCCC3C4=CC=C(C=C4)S(=O)(=O)c5ccc(Br)cc5C(F)(F)F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	603.0 (M + H)	4.60
2816	 <chem>Nc1nc2ccccc2n1C3CCCCC3C4=CC=C(C=C4)S(=O)(=O)c5cc(C(F)(F)F)cc(C(F)(F)F)c5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	577.6 (M + H)	4.72
2817	 <chem>Nc1nc2ccccc2n1C3CCCCC3C4=CC=C(C=C4)S(=O)(=O)c5c6ccccc6cc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	491 (M + H)	4.31
2818	 <chem>Nc1nc2ccccc2n1C3CCCCC3C4=CC=C(C=C4)S(=O)(=O)c5c6ccccc6cc5C(F)(F)F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	491.6 (M + H)	4.33

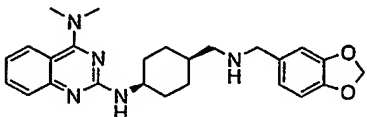
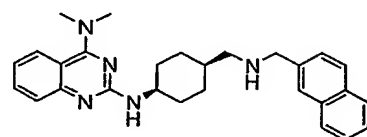
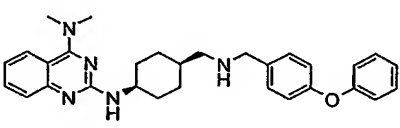
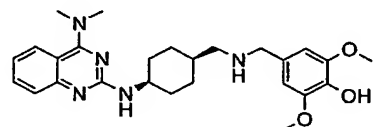
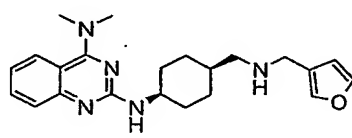
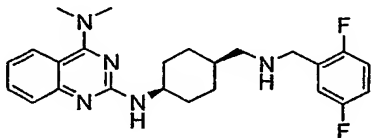
Example No.	Structure	ESI-MS	Retention Time (min)
2819	 <chem>CC1=CC=C(C=C1C(=O)NSC2CCCCC2CN3C=NC4=CC=CC=C4N3N)C5=CC=CC=C5</chem> 3CF ₃ CO ₂ H	534.6 (M + H)	4.01
2820	 <chem>NC(=N)NCC1CCCCC1CNS(=O)(=O)c2ccccc2</chem> 2HCl	325.4 (M + H)	3.91
2821	 <chem>NC(=N)NCC1CCCCC1CNS(=O)(=O)c2ccc(Cl)cc2</chem> 2HCl	359.4 (M + H)	4.24
2822	 <chem>NC(=N)NCC1CCCCC1CNS(=O)(=O)c2ccc(OC(F)(F)F)cc2</chem> 2HCl	409.4 (M + H)	4.51
2823	 <chem>CC1=CC=C(C=C1C(=O)NSC2CCCCC2CN3C=NC4=CC=CC=C4N3N)C5=CC=CC=C5</chem> 2HCl	339.6 (M + H)	4.09
2824	 <chem>BrC1=CC=C(C=C1C(=O)NSC2CCCCC2CN3C=NC4=CC=CC=C4N3N)C5=CC=CC=C5</chem> 2HCl	403.4 (M + H)	4.28

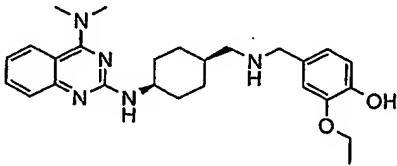
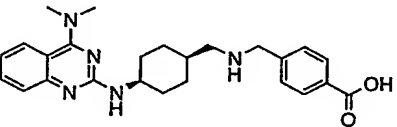
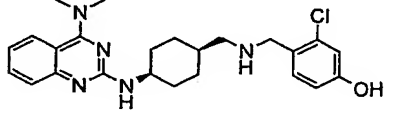
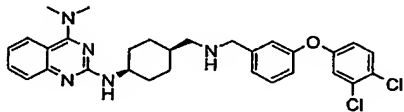
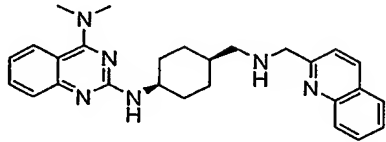
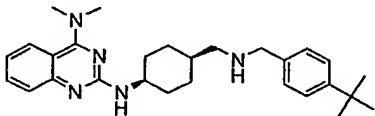
Example No.	Structure	ESI-MS	Retention Time (min)
2825	 2HCl	393.0 (M + H)	4.57
2826	 2HCl	521.6 (M + H)	4.69
2827	 2HCl	461.6 (M + H)	4.77
2828	 2HCl	375.4 (M + H)	4.33
2829	 2HCl	375.4 (M + H)	4.39
2830	 2HCl	418.8 (M + H)	4.33

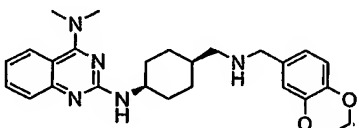
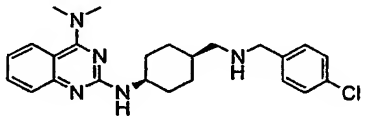
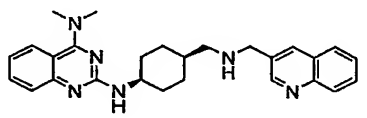
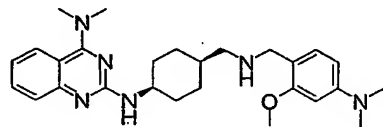
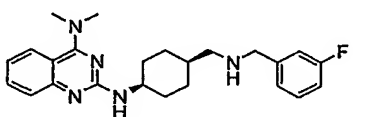
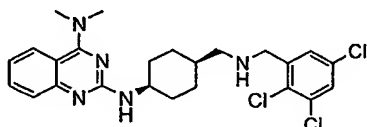
Example No.	Structure	ESI-MS	Retention Time (min)
2831	 2HCl	343.4 (M + H)	3.96
2832	 2HCl	343.4 (M + H)	4.03
2833	 2HCl	359.4 (M + H)	4.05
2834	 2HCl	359.4 (M + H)	4.24
2835	 2HCl	403.4 (M + H)	4.07
2836	 2HCl	385.4 (M + H)	4.00

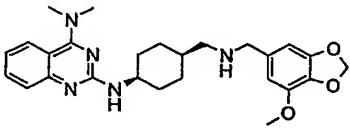
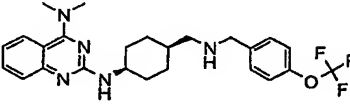
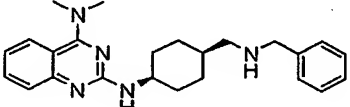
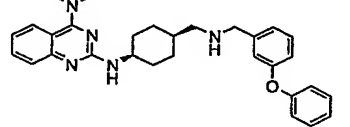
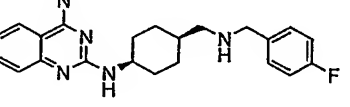
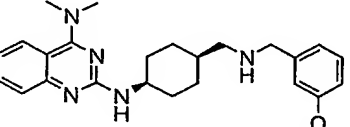
Example No.	Structure	ESI-MS	Retention Time (min)
2837	 2HCl	409.4 (M + H)	4.32
2838	 2HCl	393.6 (M + H)	4.23
2839	 2HCl	381.6 (M + H)	4.62
2840	 2HCl	330.8 (M + H)	3.83
2841	 2HCl	361.4 (M + H)	4.05
2842	 2HCl	427.4 (M + H)	4.51

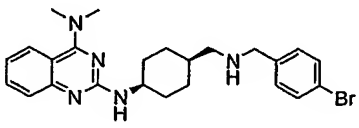
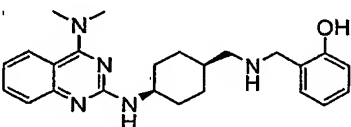
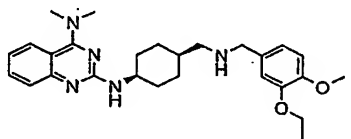
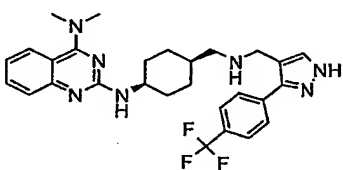
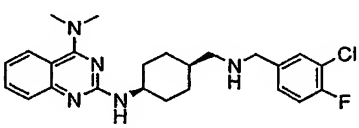
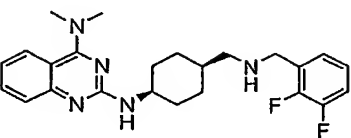
Example No.	Structure	ESI-MS	Retention Time (min)
2843	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4=CC=C(C=C4)Cl)C5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	458.4 (M + H)	3.22
2844	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4=CC=C(C=C4)C#N)C5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	415.4 (M + H)	3.01
2845	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4=CC(=C(C)C)C=C4)C5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	432.6 (M + H)	3.26
2846	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4=CC=C(C=C4)S)C5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	396.2 (M + H)	2.81
2847	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4=CC(=C(OC)OC)C=C4)C5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450.0 (M + H)	3.09
2848	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4=CC=C(C=C4)F)C5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	408.4 (M + H)	2.85

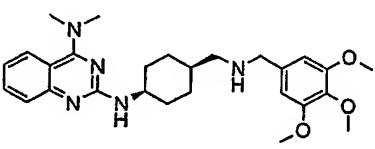
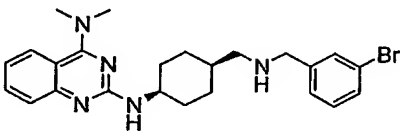
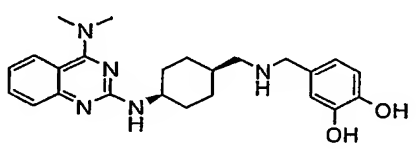
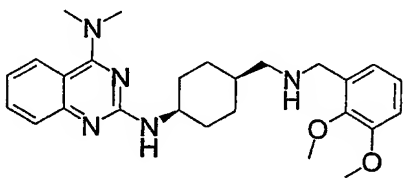
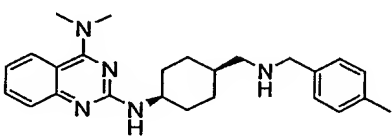
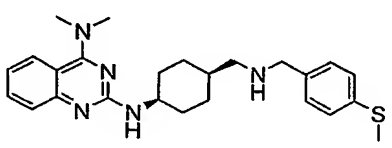
Example No.	Structure	ESI-MS	Retention Time (min)
2849	 $2\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	2.89
2850	 $2\text{CF}_3\text{CO}_2\text{H}$	440.0 (M + H)	3.20
2851	 $2\text{CF}_3\text{CO}_2\text{H}$	482.4 (M + H)	3.43
2852	 $2\text{CF}_3\text{CO}_2\text{H}$	466.4 (M + H)	2.71
2853	 $2\text{CF}_3\text{CO}_2\text{H}$	380.2 (M + H)	2.72
2854	 $2\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	2.91

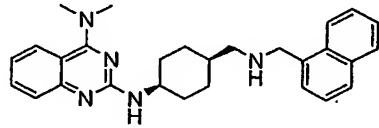
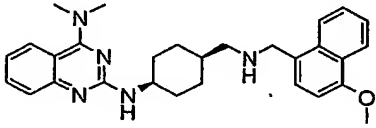
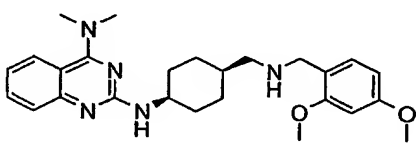
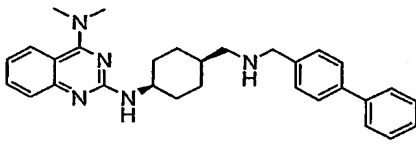
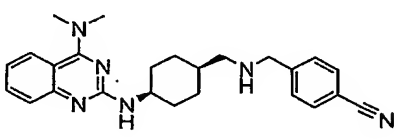
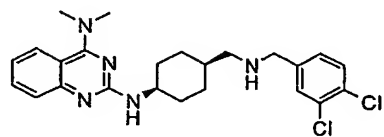
Example No.	Structure	ESI-MS	Retention Time (min)
2855	 <chem>CCOC1=CC=C(C=C1CNC2CCCCC2N3C=NC(=C4C=CC=CC=C4N3C)C)O</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450.0 (M + H)	2.82
2856	 <chem>OC(=O)C1=CC=C(C=C1CNC2CCCCC2N3C=NC(=C4C=CC=CC=C4N3C)C)C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	2.69
2857	 <chem>ClC1=CC=C(C=C1CNC2CCCCC2N3C=NC(=C4C=CC=CC=C4N3C)C)O</chem> $2\text{CF}_3\text{CO}_2\text{H}$	440.0 (M + H)	2.85
2858	 <chem>COc1cc(Cl)cc(OC1=CC=C(C=C1CNC2CCCCC2N3C=NC(=C4C=CC=CC=C4N3C)C)c1Cl</chem> $2\text{CF}_3\text{CO}_2\text{H}$	550.6 (M + H)	3.80
2859	 <chem>C1=CC=C2C(=C1)N=CN=C2C3CCCCC3N4C=NC(=C5C=CC=CC=C5N4)C</chem> $3\text{CF}_3\text{CO}_2\text{H}$	441.4 (M + H)	3.03
2860	 <chem>CC(C)(C)C1=CC=C(C=C1CNC2CCCCC2N3C=NC(=C4C=CC=CC=C4N3C)C)C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	446.6 (M + H)	3.41

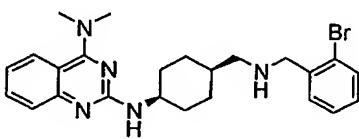
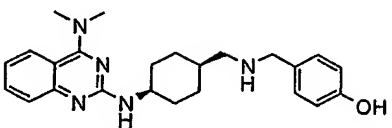
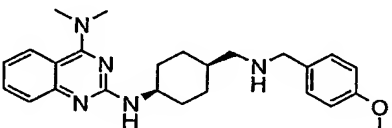
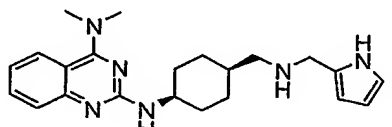
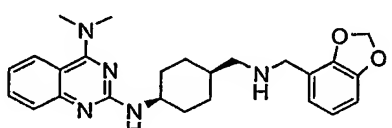
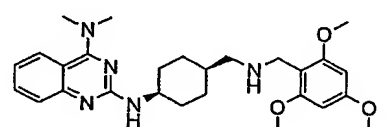
Example No.	Structure	ESI-MS	Retention Time (min)
2861	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4C=CC5C=C(C=C4)OCC5)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	2.91
2862	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4C=CC=C(C=C4)Cl)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	3.05
2863	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4C=CC5C=CC=CC=C5N4)N</chem> $3\text{CF}_3\text{CO}_2\text{H}$	441.4 (M + H)	2.68
2864	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4C=CC(OC)=C(C=C4)N(C)C</chem> $3\text{CF}_3\text{CO}_2\text{H}$	463.4 (M + H)	2.76
2865	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4C=CC=C(C=C4)F)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	408.4 (M + H)	2.91
2866	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4C=CC(=C(C=C4)Cl)Cl)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	492.2 (M + H)	3.30

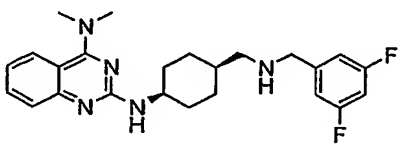
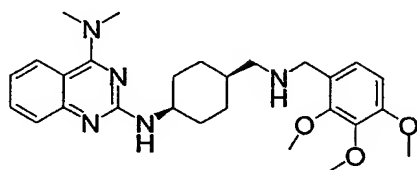
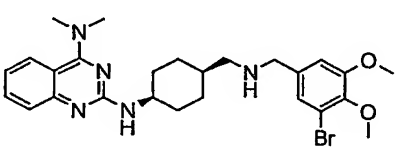
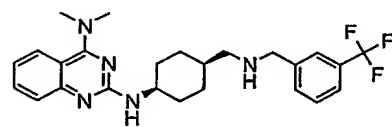
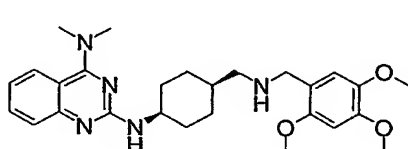
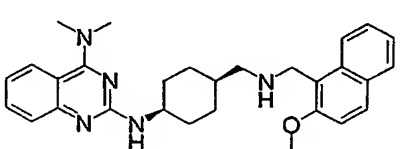
Example No.	Structure	ESI-MS	Retention Time (min)
2867	 <chem>CN(C)c1nc2c(ncn2C1)NCC3CCCCC3NCC4=CC(OC)=CC(OC)=C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	464.2 (M + H)	2.93
2868	 <chem>CN(C)c1nc2c(ncn2C1)NCC3CCCCC3NCC4=CC(OC(F)(F)F)=CC=C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	3.27
2869	 <chem>CN(C)c1nc2c(ncn2C1)NCC3CCCCC3NCC4=CC=CC=C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	390.6 (M + H)	2.88
2870	 <chem>CN(C)c1nc2c(ncn2C1)NCC3CCCCC3NCC4=CC(OC5=CC=CC=C5)=CC=C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	482.2 (M + H)	3.43
2871	 <chem>CN(C)c1nc2c(ncn2C1)NCC3CCCCC3NCC4=CC(F)=CC=C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	408.4 (M + H)	2.91
2872	 <chem>CN(C)c1nc2c(ncn2C1)NCC3CCCCC3NCC4=CC(OC)=CC=C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.91

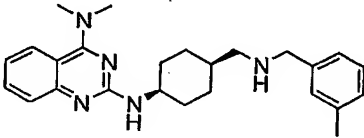
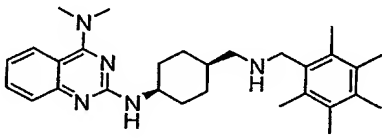
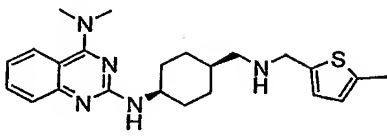
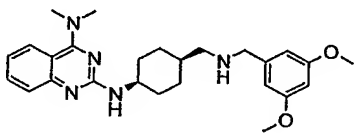
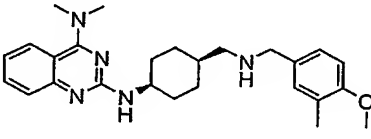
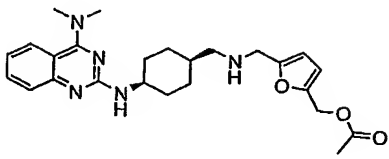
Example No.	Structure	ESI-MS	Retention Time (min)
2873	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4ccc(Br)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	468.2 (M + H)	3.09
2874	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4ccccc4O</chem> $2\text{CF}_3\text{CO}_2\text{H}$	406.4 (M + H)	2.80
2875	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4ccc(OC)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	464.2 (M + H)	2.97
2876	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4ccc(C(F)(F)F)cc4</chem> $3\text{CF}_3\text{CO}_2\text{H}$	524.6 (M + H)	3.12
2877	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc(F)ccc4Cl</chem> $2\text{CF}_3\text{CO}_2\text{H}$	442.4 (M + H)	3.10
2878	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc(F)c(F)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	2.90

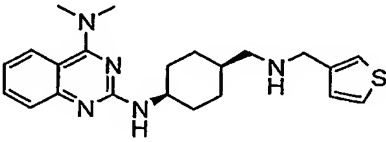
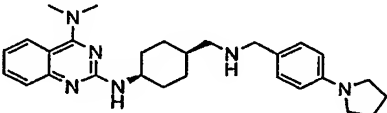
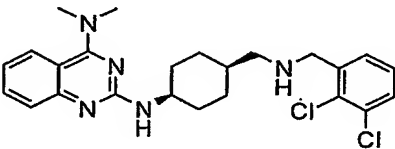
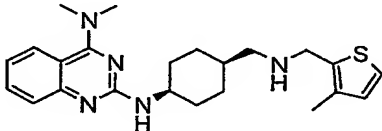
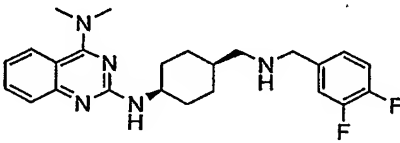
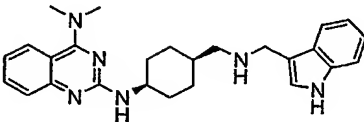
Exemplé No.	Structure	ESI-MS	Retention Time (min)
2879	 <chem>COc1cc(OC)c(OC)cc1NCC2CCCCC2Nc3nc4ccccc4n3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	480.2 (M + H)	2.89
2880	 <chem>BrC1=CC=C(C=C1)NCC2CCCCC2Nc3nc4ccccc4n3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	468.2 (M + H)	3.07
2881	 <chem>Oc1cc(O)ccc1NCC2CCCCC2Nc3nc4ccccc4n3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	422.4 (M + H)	2.61
2882	 <chem>COc1cc(OC)ccc1NCC2CCCCC2Nc3nc4ccccc4n3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450.0 (M + H)	2.93
2883	 <chem>CC1=CC=C(C=C1)NCC2CCCCC2Nc3nc4ccccc4n3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	404.6 (M + H)	3.01
2884	 <chem>CC1=CC=C(C=C1)NCC2CCCCC2Nc3nc4ccccc4n3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	3.08

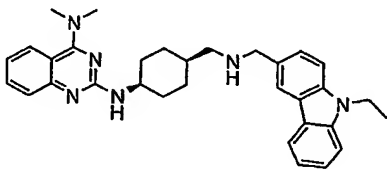
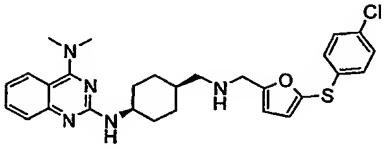
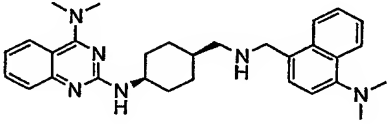
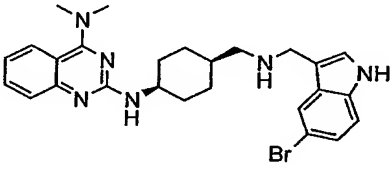
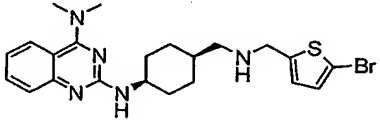
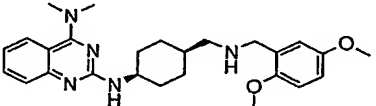
Example No.	Structure	ESI-MS	Retention Time (min)
2885	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3NCCc4c5ccccc5cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	440.0 (M + H)	3.18
2886	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3NCCc4c5cc(OC)ccc5cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	470.4 (M + H)	3.25
2887	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3NCCc4c5cc(OC)ccc(OC)c5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450.0 (M + H)	3.01
2888	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3NCCc4ccc(cc4)-c5ccccc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	466.4 (M + H)	3.40
2889	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3NCCc4ccc(cc4)C#N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	415.4 (M + H)	2.83
2890	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3NCCc4cc(Cl)c(Cl)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	458.4 (M + H)	3.25

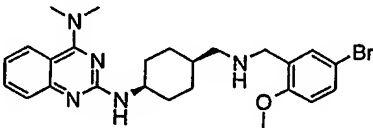
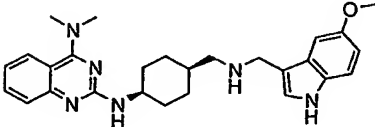
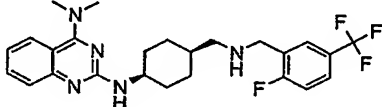
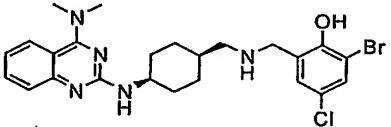
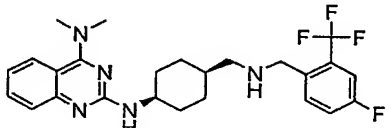
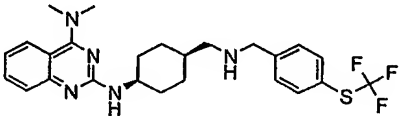
Example No.	Structure	ESI-MS	Retention Time (min)
2891	 $2\text{CF}_3\text{CO}_2\text{H}$	468.2 (M + H)	3.00
2892	 $2\text{CF}_3\text{CO}_2\text{H}$	406.4 (M + H)	2.66
2893	 $2\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.92
2894	 $3\text{CF}_3\text{CO}_2\text{H}$	379.4 (M + H)	2.71
2895	 $2\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	2.87
2896	 $2\text{CF}_3\text{CO}_2\text{H}$	480.2 (M + H)	3.17

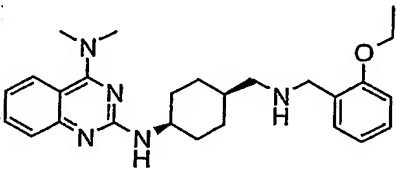
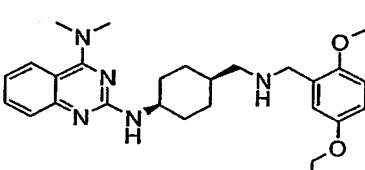
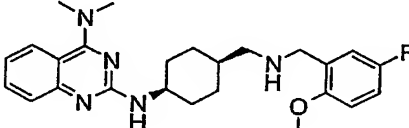
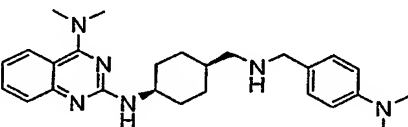
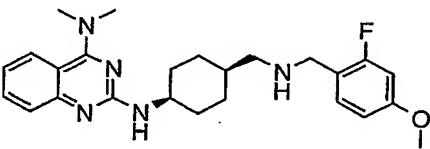
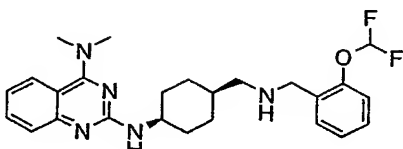
Example No.	Structure	ESI-MS	Retention Time (min)
2897	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CNCCc4ccc(F)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	2.98
2898	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CNCCc4cc(OC)c(OC)c(OC)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	480.2 (M + H)	2.99
2899	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CNCCc4cc(OC)c(Br)c(OC)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	528.4 (M + H)	3.15
2900	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CNCCc4ccc(F)(F)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	458.4 (M + H)	3.19
2901	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CNCCc4cc(OC)c(OC)c(OC)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	480.2 (M + H)	2.92
2902	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CNCCc4cc(OC)ccc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	470.4 (M + H)	3.27

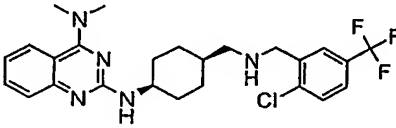
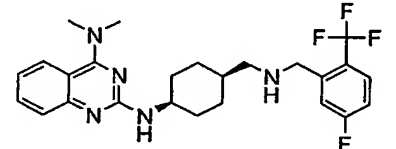
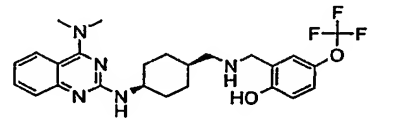
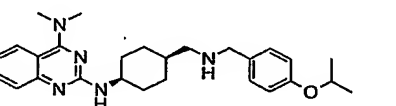
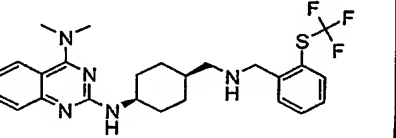
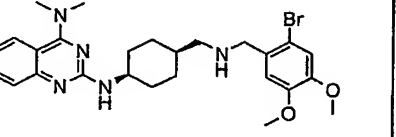
Example No.	Structure	ESI-MS	Retention Time (min)
2903	 <chem>CC1=NC2=CC=CC=C2N(C)N1CNC3CCCCC3CNCC4=CC=C(C)C=C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	404.6 (M + H)	2.87
2904	 <chem>CC1=NC2=CC=CC=C2N(C)N1CNC3CCCCC3CNCC4=C(C)C(C)=CC(C)=C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	460.4 (M + H)	3.48
2905	 <chem>CC1=NC2=CC=CC=C2N(C)N1CNC3CCCCC3CNCC4=C(C)SC=C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	410.4 (M + H)	2.96
2906	 <chem>COc1cc(CNCC2CCCCC2CNC3=NC4=CC=CC=C4N(C)N3)c(OC)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450.0 (M + H)	3.03
2907	 <chem>COc1cccc(CNCC2CCCCC2CNC3=NC4=CC=CC=C4N(C)N3)c1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	3.08
2908	 <chem>CC(=O)OCc1cc(CNCC2CCCCC2CNC3=NC4=CC=CC=C4N(C)N3)oc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	452.2 (M + H)	2.79

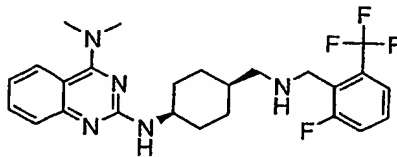
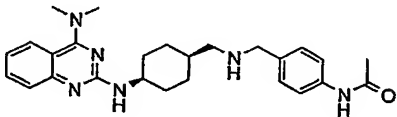
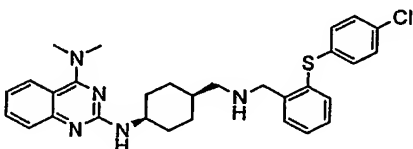
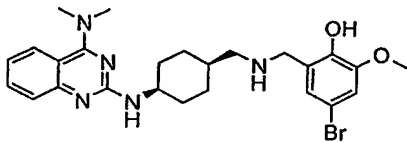
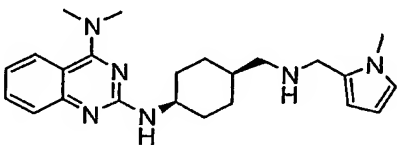
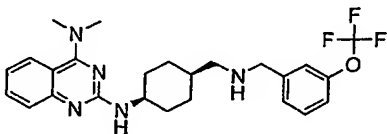
Example No.	Structure	ESI-MS	Retention Time (min)
2909	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CNCCc4ccsc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	396.2 (M + H)	2.81
2910	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CNCCc4ccc(cc4)N5CCCC5</chem> $3\text{CF}_3\text{CO}_2\text{H}$	459.4 (M + H)	3.21
2911	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CNCCc4cc(Cl)c(Cl)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	3.08
2912	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CNCCc4cc(C)cs4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	410.4 (M + H)	2.88
2913	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CNCCc4cc(F)c(F)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	3.01
2914	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CNCCc4c[nH]c5ccccc45</chem> $3\text{CF}_3\text{CO}_2\text{H}$	429.4 (M + H)	2.97

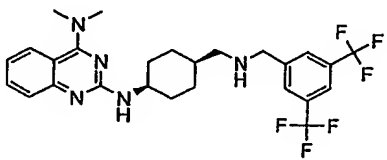
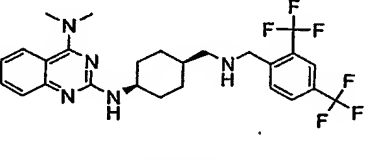
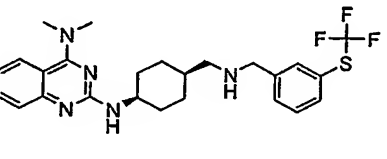
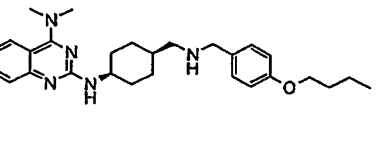
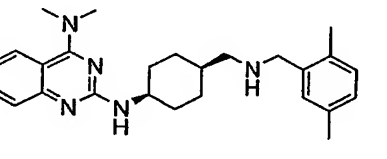
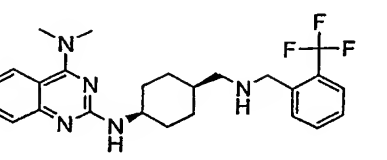
Example No.	Structure	ESI-MS	Retention Time (min)
2915	 <chem>CC1=CN2C=CC=CC=C2N1C3CCCCC3CN4C=CC5=CC=CC=C5N4C</chem> $3\text{CF}_3\text{CO}_2\text{H}$	507.2 (M + H)	3.53
2916	 <chem>Clc1ccc(SC2=CC=CC=C2O2)CCN3CCCCC3N4C=CC5=CC=CC=C5N4C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	522.4 (M + H)	3.56
2917	 <chem>CN1C=CC2=CC=CC=C2N1C3CCCCC3CN4C=CC5=CC=CC=C5N4C</chem> $3\text{CF}_3\text{CO}_2\text{H}$	483.2 (M + H)	2.80
2918	 <chem>Brc1ccc2c(c1)c(c[nH]2)CCN3CCCCC3N4C=CC5=CC=CC=C5N4C</chem> $3\text{CF}_3\text{CO}_2\text{H}$	507.2 (M + H)	3.27
2919	 <chem>Brc1ccsc1CCN2CCCCC2N3C=CC4=CC=CC=C4N3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	474.2 (M + H)	3.10
2920	 <chem>COc1cc(OC)ccc1CCN2CCCCC2N3C=CC4=CC=CC=C4N3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450.0 (M + H)	3.00

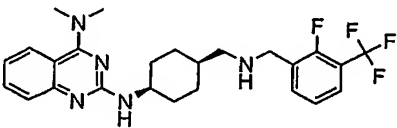
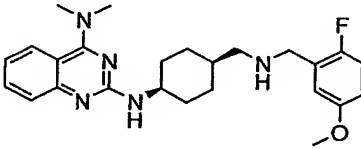
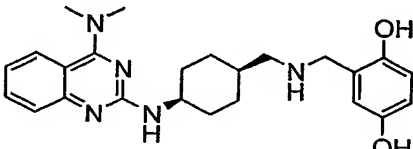
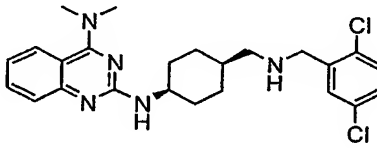
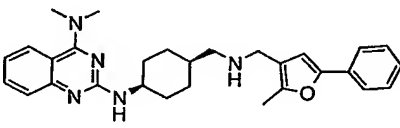
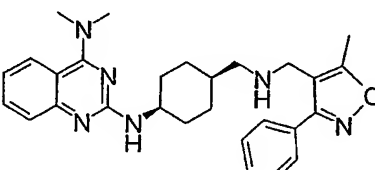
Example No.	Structure	ESI-MS	Retention Time (min)
2921	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NC4C=CC(OC)=CC=C4Br</chem> $2\text{CF}_3\text{CO}_2\text{H}$	498.4 (M + H)	3.15
2922	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NC4C=C5C(OC)C=CC=C5N4</chem> $3\text{CF}_3\text{CO}_2\text{H}$	459.4 (M + H)	2.99
2923	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NC4C=CC(F)=CC=C4F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	476.0 (M + H)	3.10
2924	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NC4C=CC(=C(C=C4)Br)O</chem> $2\text{CF}_3\text{CO}_2\text{H}$	518.2 (M + H)	3.10
2925	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NC4C=CC(F)=CC(F)=C4F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	3.12
2926	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NC4C=CC(S(=O)(=O)F)=CC=C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	3.35

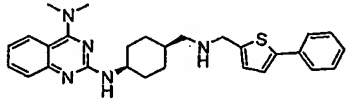
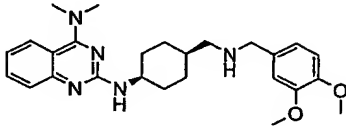
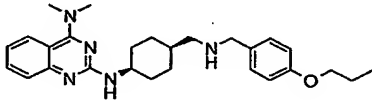
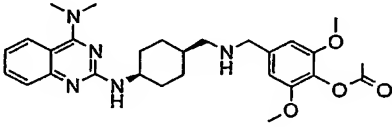
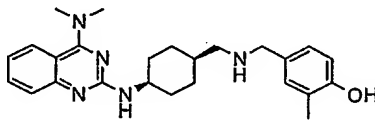
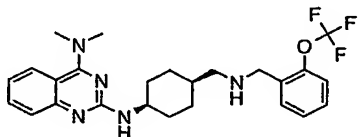
Exemplé No.	Structure	ESI-MS	Retention Time (min)
2927	 <chem>CCOC1=CC=C(C=C1)CNCC2(C)CC[C@H](N2)Nc3nc4ccccc4n3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	3.11
2928	 <chem>CCOC1=CC(=CC(=C1)OCC)NCC2(C)CC[C@H](N2)Nc3nc4ccccc4n3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	478.4 (M + H)	3.29
2929	 <chem>COc1cc(F)ccc1NCC2(C)CC[C@H](N2)Nc3nc4ccccc4n3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	438.2 (M + H)	3.01
2930	 <chem>CN(C)C1=CC=C(C=C1)NCC2(C)CC[C@H](N2)Nc3nc4ccccc4n3</chem> $3\text{CF}_3\text{CO}_2\text{H}$	433.4 (M + H)	2.59
2931	 <chem>COc1cc(F)ccc1NCC2(C)CC[C@H](N2)Nc3nc4ccccc4n3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	438.2 (M + H)	2.90
2932	 <chem>Fc1cc(OC(F)F)ccc1NCC2(C)CC[C@H](N2)Nc3nc4ccccc4n3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	456.2 (M + H)	3.10

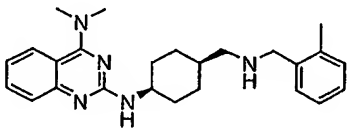
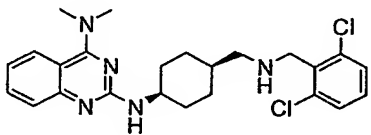
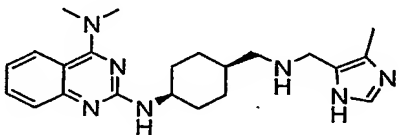
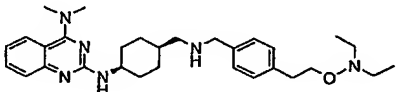
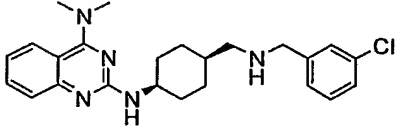
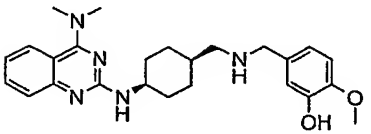
Example No.	Structure	ESI-MS	Retention Time (min)
2933	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3CN[C@@H](Cc4ccc(C(F)(F)F)cc4Cl)C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	492.2 (M + H)	3.25
2934	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3CN[C@@H](Cc4cc(F)c(F)cc4)C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	3.11
2935	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3CN[C@@H](Cc4cc(OC(F)(F)F)ccc4O)C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	3.20
2936	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3CN[C@@H](Cc4ccc(OC(C)C)cc4)C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	3.17
2937	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3CN[C@@H](Cc4ccc(SC(F)(F)F)cc4)C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	489.6 (M + H)	3.31
2938	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3CN[C@@H](Cc4cc(OC)c(Br)c(OC)c4)C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	528.2 (M + H)	3.03

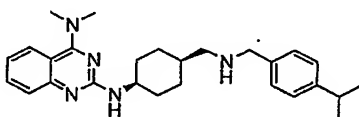
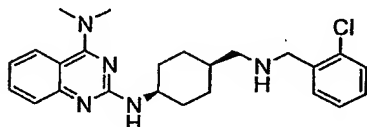
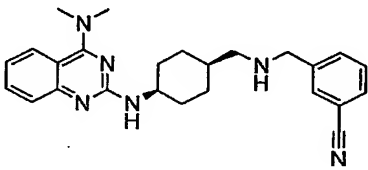
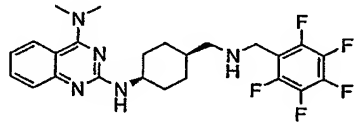
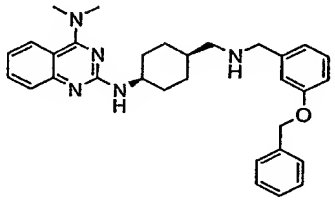
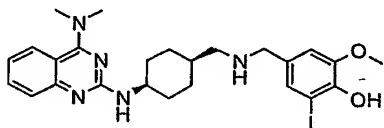
Example No.	Structure	ESI-MS	Retention Time (min)
2939	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3CN4C=CC(=C(C(F)(F)F)C(F)(F)F)C=C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	2.99
2940	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3CN4C=CC(=CC=C4)NC(=O)C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	447.4 (M + H)	2.66
2941	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3CN4C=CC(=CC=C4)SC5=CC=C(C=C5)C6=CC=CC=C6Cl</chem> $2\text{CF}_3\text{CO}_2\text{H}$	532.4 (M + H)	3.66
2942	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3CN4C=CC(=CC=C4)C(=C5C=C(C=C5)OC)Br</chem> $2\text{CF}_3\text{CO}_2\text{H}$	514.4 (M + H)	3.08
2943	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3CN4C=CC(=CC=C4)CN5C=CC=C5N5C</chem> $3\text{CF}_3\text{CO}_2\text{H}$	393.4 (M + H)	2.79
2944	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3CN4C=CC(=CC=C4)C(F)(F)F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	3.24

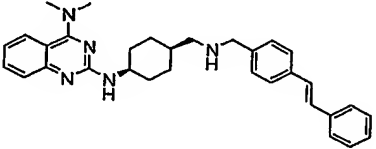
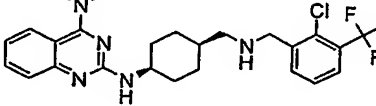
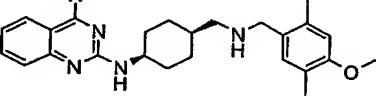
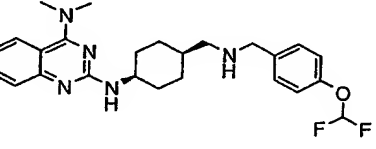
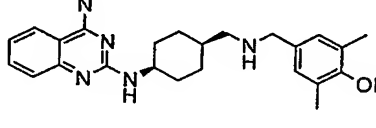
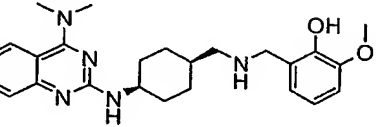
Example No.	Structure	ESI-MS	Retention Time (min)
2945	 <chem>CN(C)c1nc2ccccc2n1CN[C@H]1CCCC[C@H]1CNCCc2cc(F)c(F)c(F)c2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	526.6 (M + H)	3.44
2946	 <chem>CN(C)c1nc2ccccc2n1CN[C@H]1CCCC[C@H]1CNCCc2cc(F)c(F)c(F)c2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	526.6 (M + H)	3.42
2947	 <chem>CN(C)c1nc2ccccc2n1CN[C@H]1CCCC[C@H]1CNCCc2ccc(SC(F)(F)F)cc2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	3.35
2948	 <chem>CN(C)c1nc2ccccc2n1CN[C@H]1CCCC[C@H]1CNCCc2ccc(OCC)cc2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	3.43
2949	 <chem>CN(C)c1nc2ccccc2n1CN[C@H]1CCCC[C@H]1CNCCc2ccc(C)cc2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	3.13
2950	 <chem>CN(C)c1nc2ccccc2n1CN[C@H]1CCCC[C@H]1CNCCc2cc(F)c(F)cc2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	458.4 (M + H)	3.10

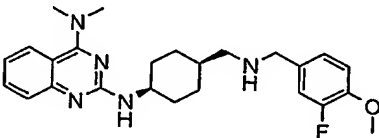
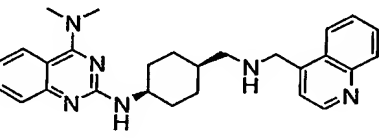
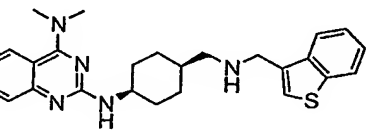
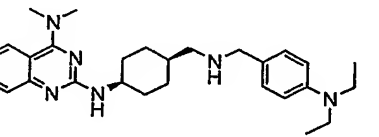
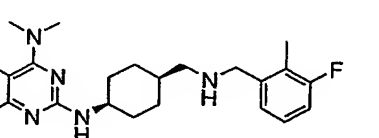
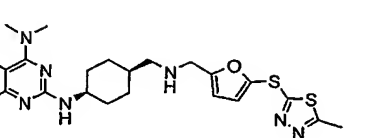
Example No.	Structure	ESI-MS	Retention Time (min)
2951	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNCCc4ccc(C(F)(F)F)cc4</chem> $2CF_3CO_2H$	476.4 (M + H)	3.19
2952	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNCCc4cc(OC)cc(F)c4</chem> $2CF_3CO_2H$	438.2 (M + H)	2.95
2953	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNCCc4cc(O)cc(O)c4</chem> $2CF_3CO_2H$	422.4 (M + H)	2.61
2954	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNCCc4cc(Cl)cc(Cl)c4</chem> $2CF_3CO_2H$	458.2 (M + H)	3.07
2955	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNCCc4cc5oc(cc5)cc4-c6ccccc6</chem> $2CF_3CO_2H$	470.4 (M + H)	3.45
2956	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNCCc4cc5ccccc5nn4</chem> $2CF_3CO_2H$	471.6 (M + H)	2.88

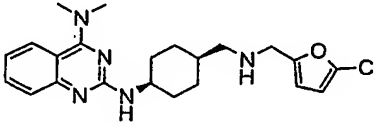
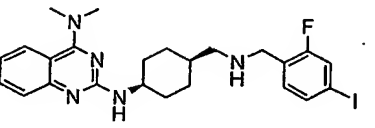
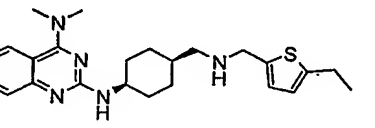
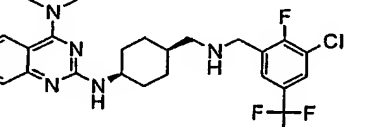
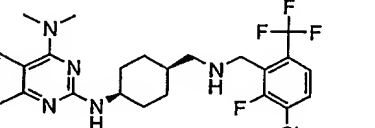
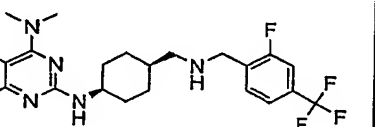
Example No.	Structure	ESI-MS	Retention Time (min)
2957	 <chem>CN1C=NC2=C(N1)C=CC=C2NCC3CCCCC3NCC4=CC=CC=C4S</chem> $2\text{CF}_3\text{CO}_2\text{H}$	472.4 (M + H)	3.36
2958	 <chem>CN1C=NC2=C(N1)C=CC=C2NCC3CCCCC3NCC4=CC(OC)=C(OC)C=C4OC</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450 (M + H)	2.75
2959	 <chem>CN1C=NC2=C(N1)C=CC=C2NCC3CCCCC3NCC4=CC=CC=C4OCC</chem> $2\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	3.20
2960	 <chem>CN1C=NC2=C(N1)C=CC=C2NCC3CCCCC3NCC4=CC(OC)=C(OC(=O)OC)C=C4OC</chem> $2\text{CF}_3\text{CO}_2\text{H}$	508.4 (M + H)	3.00
2961	 <chem>CN1C=NC2=C(N1)C=CC=C2NCC3CCCCC3NCC4=CC=CC=C4O</chem> $2\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.80
2962	 <chem>CN1C=NC2=C(N1)C=CC=C2NCC3CCCCC3NCC4=CC=C(C=C4)OC(F)(F)F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	3.20

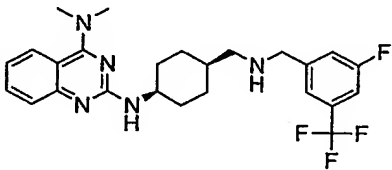
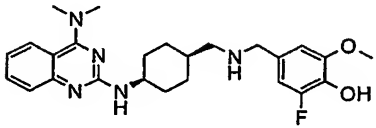
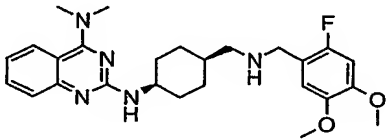
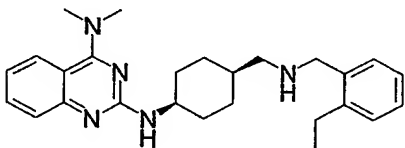
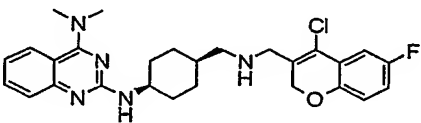
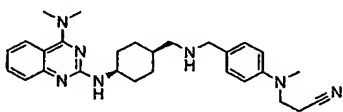
Example No.	Structure	ESI-MS	Retention Time (min)
2963	 <chem>CCN(C)c1nc2ccccc2n1NC3CCCCC3CNCC4=CC=C(C)C=C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	404.4 (M + H)	2.87
2964	 <chem>CCN(C)c1nc2ccccc2n1NC3CCCCC3CNCC4=CC(=C(C=C4)Cl)Cl</chem> $2\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	3.00
2965	 <chem>CCN(C)c1nc2ccccc2n1NC3CCCCC3CNCC4=CN=CN4</chem> $3\text{CF}_3\text{CO}_2\text{H}$	394.4 (M + H)	2.30
2966	 <chem>CCN(C)c1nc2ccccc2n1NC3CCCCC3CNCC4=CC=C(C=C4)COCCN(CC)</chem> $2\text{CF}_3\text{CO}_2\text{H}$	505.4 (M + H)	2.60
2967	 <chem>CCN(C)c1nc2ccccc2n1NC3CCCCC3CNCC4=CC=C(C=C4)Cl</chem> $2\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	3.00
2968	 <chem>CCN(C)c1nc2ccccc2n1NC3CCCCC3CNCC4=CC(=C(C=C4)O)I</chem> $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	2.71

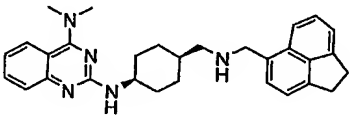
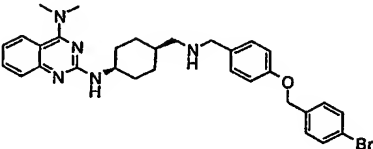
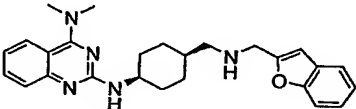
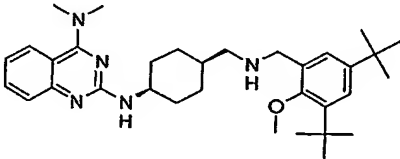
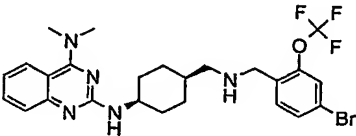
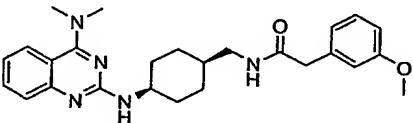
Example No.	Structure	ESI-MS	Retention Time (min)
2969	 <chem>CC(C)c1ccc(cc1)CNCC2CCCCC2Nc3nc4ccccc4n3C(C)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	432.4 (M + H)	3.30
2970	 <chem>Clc1ccc(cc1)CNCC2CCCCC2Nc3nc4ccccc4n3C(C)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	2.95
2971	 <chem>N#Cc1ccc(cc1)CNCC2CCCCC2Nc3nc4ccccc4n3C(C)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	415.4 (M + H)	2.79
2972	 <chem>Fc1cc(F)c(F)c(F)c1CNCC2CCCCC2Nc3nc4ccccc4n3C(C)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	480.2 (M + H)	3.00
2973	 <chem>c1ccc(cc1)OCc2ccc(cc2)CNCC3CCCCC3Nc4nc5ccccc5n4C(C)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	496.2 (M + H)	3.46
2974	 <chem>COc1cc(O)ccc1CNCC2CCCCC2Nc3nc4ccccc4n3C(C)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	562.2 (M + H)	2.99

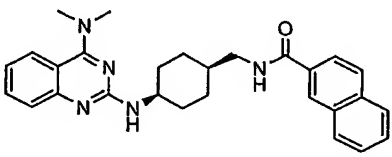
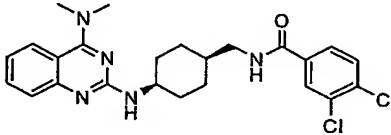
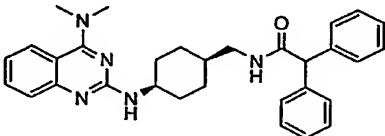
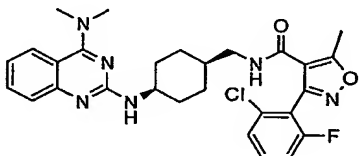
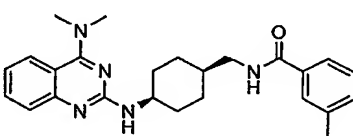
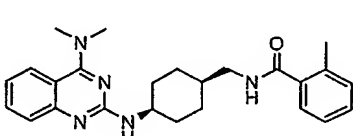
Example No.	Structure	ESI-MS	Retention Time (min)
2975	 2CF ₃ CO ₂ H	492.4 (M + H)	3.64
2976	 2CF ₃ CO ₂ H	492.2 (M + H)	3.25
2977	 2CF ₃ CO ₂ H	448.4 (M + H)	3.22
2978	 2CF ₃ CO ₂ H	456.2 (M + H)	3.09
2979	 2CF ₃ CO ₂ H	434.4 (M + H)	2.89
2980	 2CF ₃ CO ₂ H	436.4 (M + H)	2.79

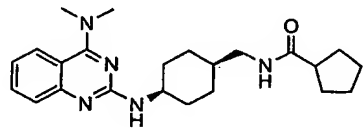
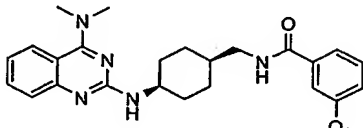
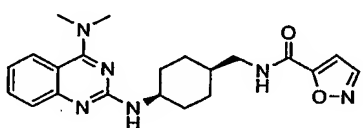
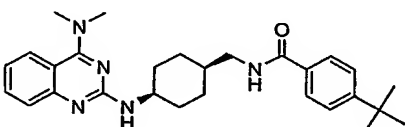
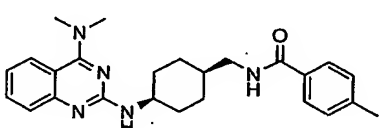
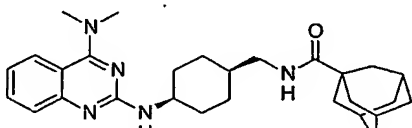
Example No.	Structure	ESI-MS	Retention Time (min)
2981	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3CNCCc4cc(OC)c(F)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	438.2 (M + H)	2.91
2982	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3CNCCc4cnc5ccccc45</chem> $3\text{CF}_3\text{CO}_2\text{H}$	441.4 (M + H)	2.55
2983	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3CNCCc4c5ccccc4s5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	446.4 (M + H)	3.13
2984	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3CNCCc4ccc(NCC)cc4</chem> $3\text{CF}_3\text{CO}_2\text{H}$	461.4 (M + H)	2.46
2985	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3CNCCc4cc(F)ccc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	422.2 (M + H)	3.01
2986	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3CNCCc4oc5c(snn5)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	510.2 (M + H)	2.85

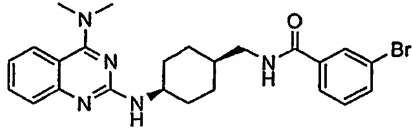
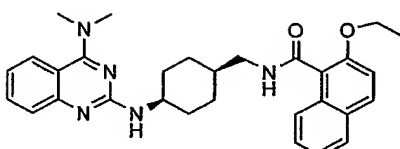
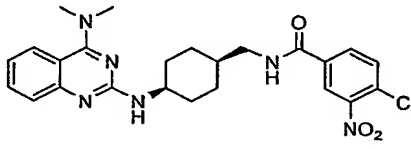
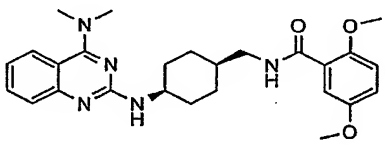
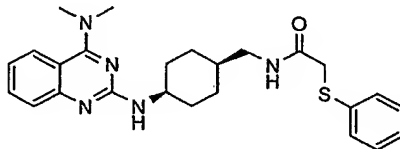
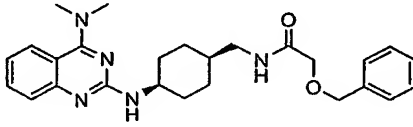
Example No.	Structure	ESI-MS	Retention Time (min)
2987	 <chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4CNCC5=CC=C(C=C5)Cl</chem> $2\text{CF}_3\text{CO}_2\text{H}$	414.4 (M + H)	2.86
2988	 <chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4CNCC5=CC=C(C=C5)F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	534.2 (M + H)	3.13
2989	 <chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4CNCC5=CC=C(C=C5)S</chem> $2\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	3.08
2990	 <chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4CNCC5=CC=C(C=C5)C(F)(F)F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	510.4 (M + H)	3.32
2991	 <chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4CNCC5=CC=C(C=C5)C(F)(F)F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	510.4 (M + H)	3.17
2992	 <chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4CNCC5=CC=C(C=C5)F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	476.4 (M + H)	3.17

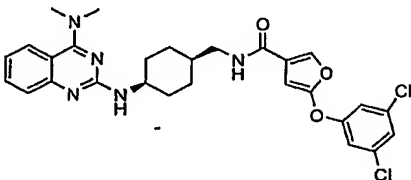
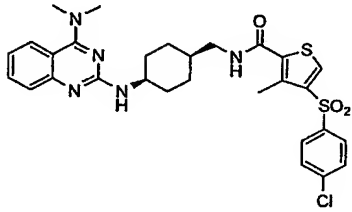
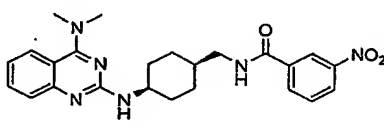
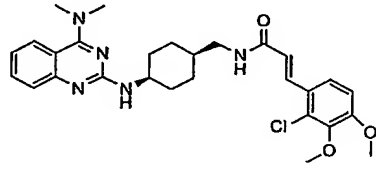
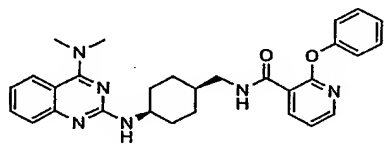
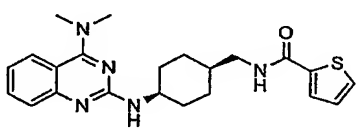
Example No.	Structure	ESI-MS	Retention Time (min)
2993	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4ccc(C(F)(F)F)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	3.21
2994	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc(OC)c(F)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	454.2 (M + H)	2.77
2995	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc(OC)c(F)c(OC)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	468.4 (M + H)	2.89
2996	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4ccccc4C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	3.12
2997	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4c5ccccc5oc4ClF</chem> $2\text{CF}_3\text{CO}_2\text{H}$	496.4 (M + H)	3.29
2998	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4ccc(CN(C)C#N)cc4</chem> $3\text{CF}_3\text{CO}_2\text{H}$	472.6 (M + H)	2.99

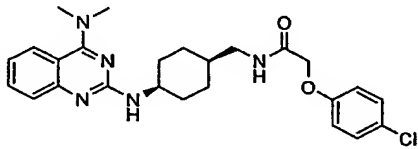
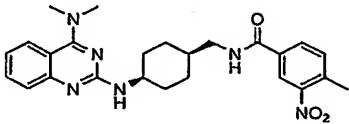
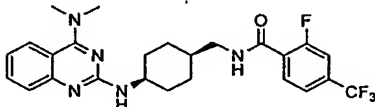
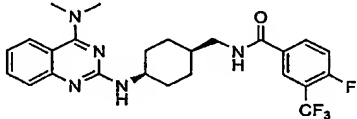
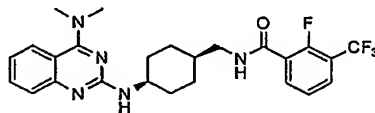
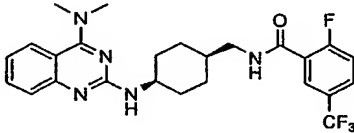
Example No.	Structure	ESI-MS	Retention Time (min)
2999	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3=CC=CC=C3N3C4CCCCC4CNC5=CC6=CC=CC=C6C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	466.4 (M + H)	3.37
3000	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3=CC=CC=C3N3C4CCCCC4CNC5=CC=C(C=C5)OC6=CC=C(C=C6)Br</chem> $2\text{CF}_3\text{CO}_2\text{H}$	574.2 (M + H)	3.64
3001	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3=CC=CC=C3N3C4CCCCC4CNC5=CC6=C(C=C5)OC7=CC=CC=C76</chem> $2\text{CF}_3\text{CO}_2\text{H}$	430.4 (M + H)	3.05
3002	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3=CC=CC=C3N3C4CCCCC4CNC5=CC(=C(C=C5)OC)C(C)=C(C)C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	532.4 (M + H)	4.05
3003	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3=CC=CC=C3N3C4CCCCC4CNC5=CC(=C(C=C5)OC(F)(F)F)Br</chem> $2\text{CF}_3\text{CO}_2\text{H}$	552.0 (M + H)	3.37
3004	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3=CC=CC=C3N3C4CCCCC4CNC(=O)Cc5ccc(OC)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	3.51

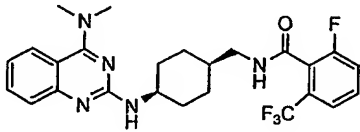
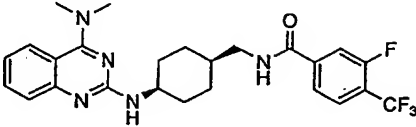
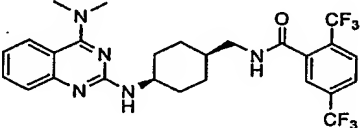
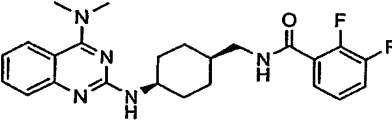
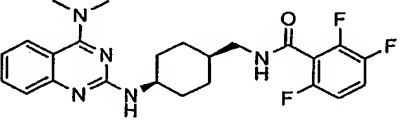
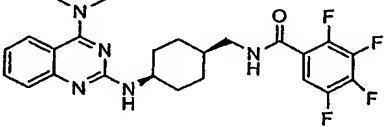
Example No.	Structure	ESI-MS	Retention Time (min)
3005	 <chem>CC1=NC2=CC=CC=C2N1C(C)C3CCCCC3NC(=O)c4c5ccccc5cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	454.2 (M + H)	3.91
3006	 <chem>CC1=NC2=CC=CC=C2N1C(C)C3CCCCC3NC(=O)c4cc(Cl)cc(Cl)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.4 (M + H)	4.02
3007	 <chem>CC1=NC2=CC=CC=C2N1C(C)C3CCCCC3NC(=O)C(c4ccccc4)c5ccccc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	494.4 (M + H)	4.01
3008	 <chem>CC1=NC2=CC=CC=C2N1C(C)C3CCCCC3NC(=O)N4C(=O)c5cc(F)ccc5N4OC</chem> $\text{CF}_3\text{CO}_2\text{H}$	537.4 (M + H)	3.77
3009	 <chem>CC1=NC2=CC=CC=C2N1C(C)C3CCCCC3NC(=O)c4cc(C)ccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	3.63
3010	 <chem>CC1=NC2=CC=CC=C2N1C(C)C3CCCCC3NC(=O)c4cc(C)ccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	3.51

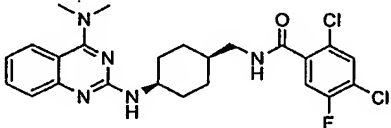
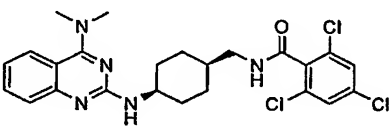
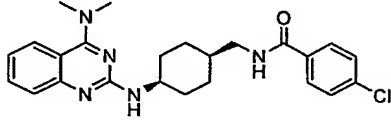
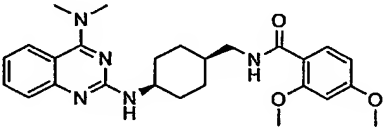
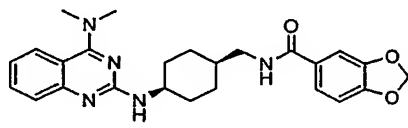
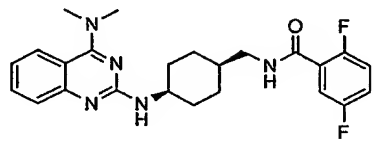
Example No.	Structure	ESI-MS	Retention Time (min)
3011	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCCCC3NC(=O)C4CCCC4</chem> <chem>CF3CO2H</chem>	396.2 (M + H)	3.47
3012	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCCCC3NC(=O)c4ccc(OC)cc4</chem> <chem>CF3CO2H</chem>	434.4 (M + H)	3.52
3013	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCCCC3NC(=O)c4ccoc4[N+]([O-])=O</chem> <chem>CF3CO2H</chem>	395.4 (M + H)	3.15
3014	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCCCC3NC(=O)c4ccc(C(C)(C)C)cc4</chem> <chem>CF3CO2H</chem>	460.2 (M + H)	4.03
3015	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCCCC3NC(=O)c4ccc(C)cc4</chem> <chem>CF3CO2H</chem>	418.6 (M + H)	3.65
3016	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCCCC3NC(=O)C4C=CC5C4C=CC5</chem> <chem>CF3CO2H</chem>	462.2 (M + H)	4.09

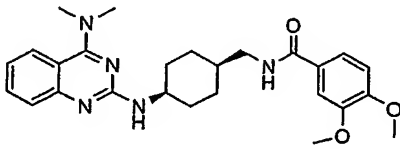
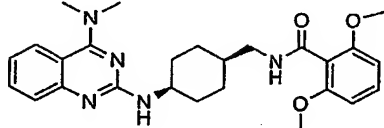
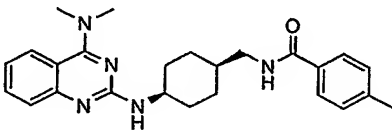
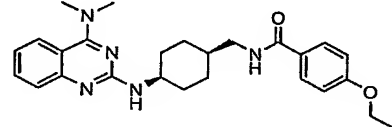
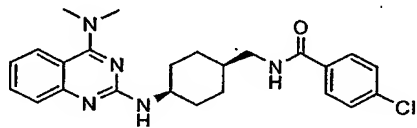
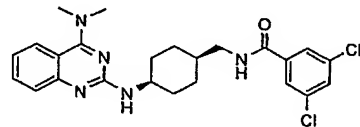
Example No.	Structure	ESI-MS	Retention Time (min)
3017	 <chem>CC1=NC2=CC=CC=C2N1N(C)C(C)N2C3CCCCC3CCNC(=O)c4ccc(Br)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	484.2 (M + H)	3.79
3018	 <chem>CC1=NC2=CC=CC=C2N1N(C)C(C)N2C3CCCCC3CCNC(=O)c4ccc(OC)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	498.6 (M + H)	3.88
3019	 <chem>CC1=NC2=CC=CC=C2N1N(C)C(C)N2C3CCCCC3CCNC(=O)c4cc([N+](=O)[O-])cc(Cl)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	483.2 (M + H)	3.80
3020	 <chem>CC1=NC2=CC=CC=C2N1N(C)C(C)N2C3CCCCC3CCNC(=O)c4cc(OC)cc(OC)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	478.2 (M + H)	3.49
3021	 <chem>CC1=NC2=CC=CC=C2N1N(C)C(C)N2C3CCCCC3CCNC(=O)CCSc4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	450.0 (M + H)	3.61
3022	 <chem>CC1=NC2=CC=CC=C2N1N(C)C(C)N2C3CCCCC3CCNC(=O)COc4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	448.2 (M + H)	3.70

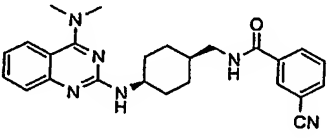
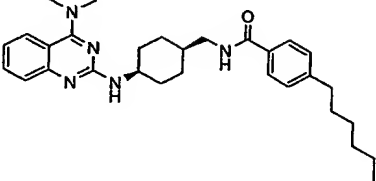
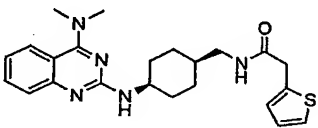
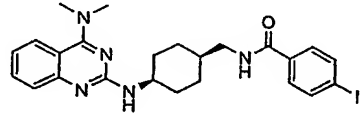
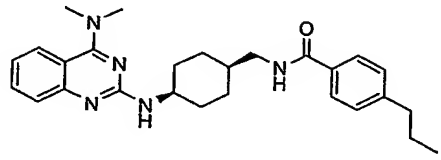
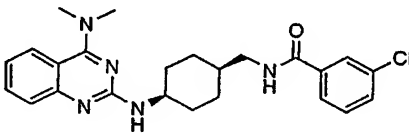
Example No.	Structure	ESI-MS	Retention Time (min)
3023	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNC(=O)c4oc(cc4)Oc5cc(Cl)cc(Cl)c5</chem> $\text{CF}_3\text{CO}_2\text{H}$	554.4 (M + H)	4.41
3024	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNC(=O)c4sc(cc4)S(=O)(=O)c5ccc(Cl)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	598.2 (M + H)	4.03
3025	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNC(=O)c4ccc([N+](=O)[O-])cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	499.2 (M + H)	3.59
3026	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNC(=O)C=Cc4cc(OC)c(Cl)c(OC)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	524.6 (M + H)	3.84
3027	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNC(=O)c4cccnc4Oc5ccccc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	497.4 (M + H)	3.80
3028	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNC(=O)c4ccsc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	410.2 (M + H)	3.43

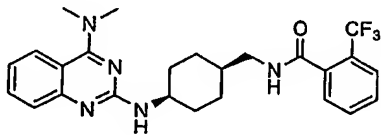
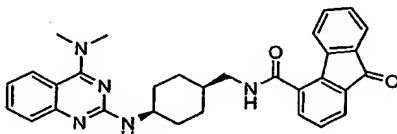
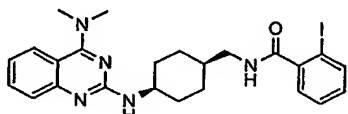
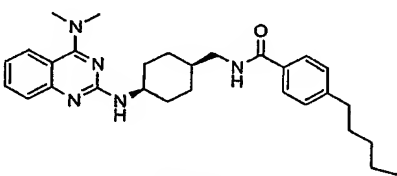
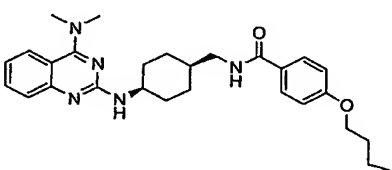
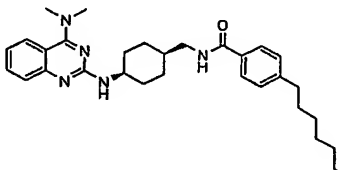
Example No.	Structure	ESI-MS	Retention Time (min)
3029	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC3CCCCC3CNC(=O)COC4=CC=C(C=C4)Cl)N2C</chem> $\text{CF}_3\text{CO}_2\text{H}$	468.2 (M + H)	3.77
3030	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC3CCCCC3CNC(=O)C4=CC=C(C=C4)[N+](=O)[O-])N2C</chem> $\text{CF}_3\text{CO}_2\text{H}$	463.2 (M + H)	3.73
3031	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC3CCCCC3CNC(=O)C4=CC(=CC=C4)C(F)=CC(F)(F)F)N2C</chem> $\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	3.91
3032	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC3CCCCC3CNC(=O)C4=CC(=CC=C4)C(F)=CC(F)(F)F)N2C</chem> $\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	3.94
3033	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC3CCCCC3CNC(=O)C4=CC(=CC=C4)C(F)=CC(F)(F)F)N2C</chem> $\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	3.85
3034	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC3CCCCC3CNC(=O)C4=CC(=CC=C4)C(F)=CC(F)(F)F)N2C</chem> $\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	3.87

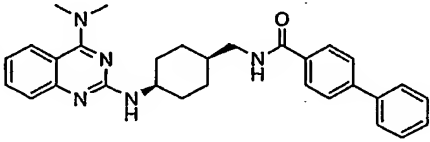
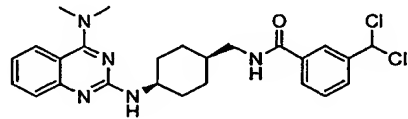
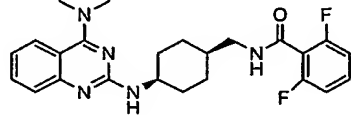
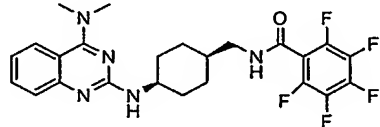
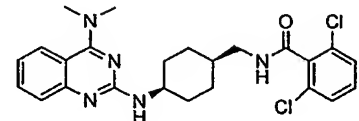
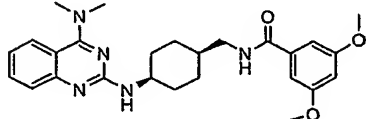
Example No.	Structure	ESI-MS	Retention Time (min)
3035	 <chem>CC1=NC2=CC=CC=C2N1C3CCCCC3CCNC(=O)c4cc(F)cc(C(F)(F)F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	3.63
3036	 <chem>CC1=NC2=CC=CC=C2N1C3CCCCC3CCNC(=O)c4cc(F)c(C(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	490.2 (M + H)	3.54
3037	 <chem>CC1=NC2=CC=CC=C2N1C3CCCCC3CCNC(=O)c4cc(C(F)(F)F)cc(C(F)(F)F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	540.4 (M + H)	3.95
3038	 <chem>CC1=NC2=CC=CC=C2N1C3CCCCC3CCNC(=O)c4cc(F)c(F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.4 (M + H)	3.58
3039	 <chem>CC1=NC2=CC=CC=C2N1C3CCCCC3CCNC(=O)c4cc(F)cc(F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.4 (M + H)	3.56
3040	 <chem>CC1=NC2=CC=CC=C2N1C3CCCCC3CCNC(=O)c4cc(F)c(F)c(F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.4 (M + H)	3.83

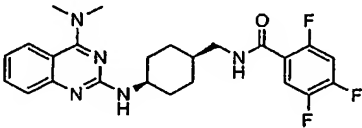
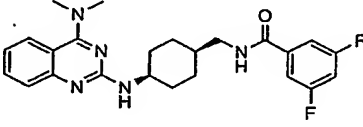
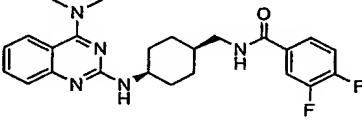
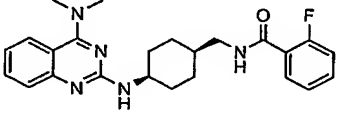
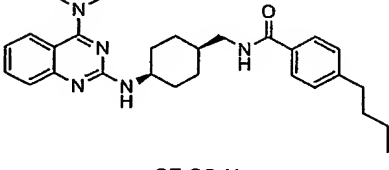
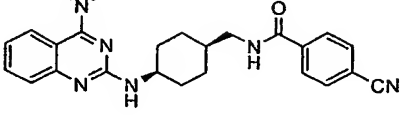
Example No.	Structure	ESI-MS	Retention Time (min)
3041	 <chem>CC1=NC2=CC=CC=C2N1C(C)N[C@H]3CCCC[C@H]3CNC(=O)c1cc(Cl)cc(F)c1</chem> <chem>CF3CO2H</chem>	490.4 (M + H)	3.82
3042	 <chem>CC1=NC2=CC=CC=C2N1C(C)N[C@H]3CCCC[C@H]3CNC(=O)c1cc(Cl)c(Cl)c(Cl)c1</chem> <chem>CF3CO2H</chem>	508.0 (M + H)	3.85
3043	 <chem>CC1=NC2=CC=CC=C2N1C(C)N[C@H]3CCCC[C@H]3CNC(=O)c1ccc(Cl)cc1</chem> <chem>CF3CO2H</chem>	438.2 (M + H)	3.71
3044	 <chem>CC1=NC2=CC=CC=C2N1C(C)N[C@H]3CCCC[C@H]3CNC(=O)c1cc(OC)cc(OC)c1</chem> <chem>CF3CO2H</chem>	464.2 (M + H)	3.65
3045	 <chem>CC1=NC2=CC=CC=C2N1C(C)N[C@H]3CCCC[C@H]3CNC(=O)c1ccc2occc2c1</chem> <chem>CF3CO2H</chem>	448.4 (M + H)	3.47
3046	 <chem>CC1=NC2=CC=CC=C2N1C(C)N[C@H]3CCCC[C@H]3CNC(=O)c1cc(F)cc(F)c1</chem> <chem>CF3CO2H</chem>	440.4 (M + H)	3.59

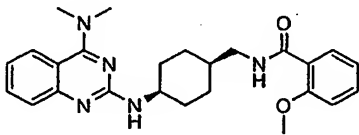
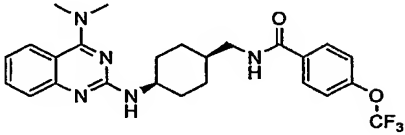
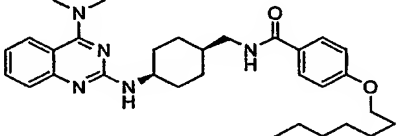
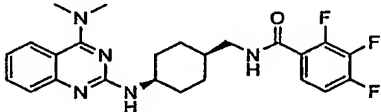
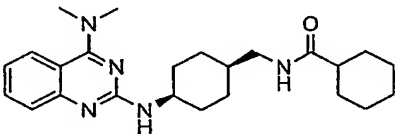
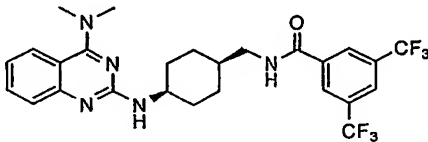
Example No.	Structure	ESI-MS	Retention Time (min)
3047	 <chem>COc1cc(OC)c(NC(=O)C2CCC(CC2)Nc3nc4ccccc4n3C)cc1OC</chem> $\text{CF}_3\text{CO}_2\text{H}$	464.2 (M + H)	3.36
3048	 <chem>COc1cc(NC(=O)C2CCC(CC2)Nc3nc4ccccc4n3C)c(OC)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	3.39
3049	 <chem>CCC1=CC=C(NC(=O)C2CCC(CC2)Nc3nc4ccccc4n3C)C=C1</chem> $\text{CF}_3\text{CO}_2\text{H}$	432.4 (M + H)	3.81
3050	 <chem>COc1ccc(NC(=O)C2CCC(CC2)Nc3nc4ccccc4n3C)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	3.69
3051	 <chem>Clc1ccc(NC(=O)C2CCC(CC2)Nc3nc4ccccc4n3C)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	438.2 (M + H)	3.69
3052	 <chem>Clc1cc(NC(=O)C2CCC(CC2)Nc3nc4ccccc4n3C)cc(Cl)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.4 (M + H)	4.03

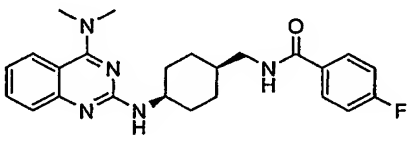
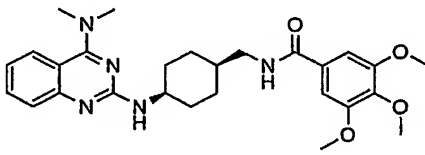
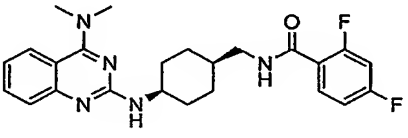
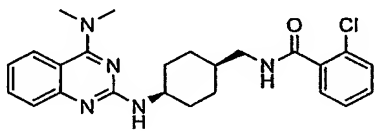
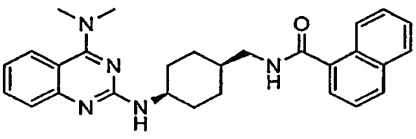
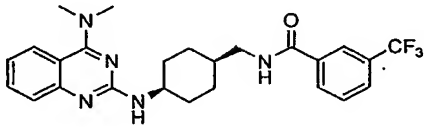
Example No.	Structure	ESI-MS	Retention Time (min)
3053	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC(=O)C4=CC=C(C#N)C=C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	429.2 (M + H)	3.47
3054	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC(=O)C4=CC=C(CCCC)C=C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	488.4 (M + H)	4.60
3055	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC(=O)CS4=CC=CC=C4S</chem> $\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	3.41
3056	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC(=O)C4=CC=C(I)C=C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	530.2 (M + H)	3.83
3057	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC(=O)C4=CC=C(CCC)C=C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	446.4 (M + H)	4.02
3058	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC(=O)C4=CC=C(Cl)C=C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	438.2 (M + H)	3.70

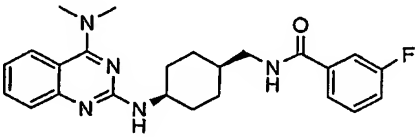
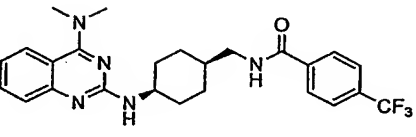
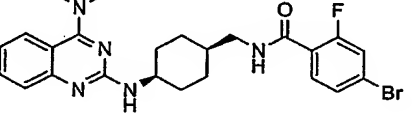
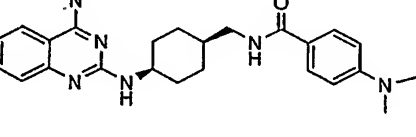
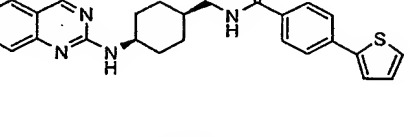
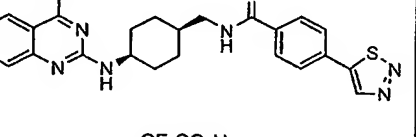
Example No.	Structure	ESI-MS	Retention Time (min)
3059	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N2C3CCCCC3CC(=O)Nc4ccc(C(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.4 (M + H)	3.55
3060	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N2C3CCCCC3CC(=O)Nc4c5ccccc4C(=O)c6ccccc56</chem> $\text{CF}_3\text{CO}_2\text{H}$	506.4 (M + H)	3.71
3061	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N2C3CCCCC3CC(=O)Nc4ccc(I)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	530.2 (M + H)	3.61
3062	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N2C3CCCCC3CC(=O)Nc4ccc(CCCCC)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	4.41
3063	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N2C3CCCCC3CC(=O)Nc4ccc(OCC)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.4 (M + H)	4.14
3064	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N2C3CCCCC3CC(=O)Nc4ccc(CCCCCC)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	502.4 (M + H)	4.83

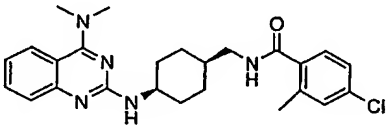
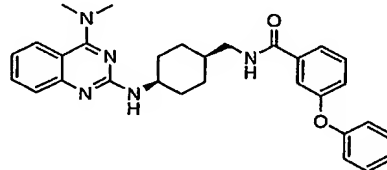
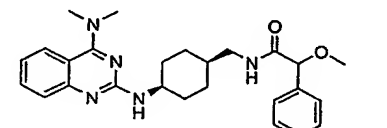
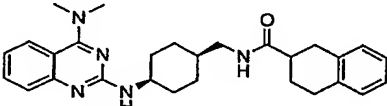
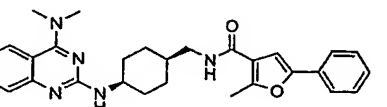
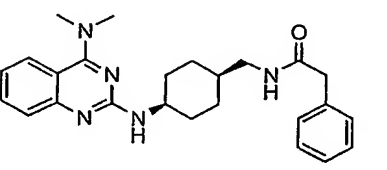
Example No:	Structure	ESI-MS	Retention Time (min)
3065	 <chem>CC1=NC2=CC=CC=C2N(C)N1C3=CC=CC=C3NC(=O)C4=CC=CC=C4C5=CC=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	480.4 (M + H)	4.09
3066	 <chem>CC1=NC2=CC=CC=C2N(C)N1C3=CC=CC=C3NC(=O)C4=CC=CC=C4CC5(Cl)C(Cl)C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	486.4 (M + H)	3.84
3067	 <chem>CC1=NC2=CC=CC=C2N(C)N1C3=CC=CC=C3NC(=O)C4=CC(=CC=C4)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.4 (M + H)	3.46
3068	 <chem>CC1=NC2=CC=CC=C2N(C)N1C3=CC=CC=C3NC(=O)C4=CC(F)=C(F)C(F)=C4F</chem> $\text{CF}_3\text{CO}_2\text{H}$	494.4 (M + H)	3.79
3069	 <chem>CC1=NC2=CC=CC=C2N(C)N1C3=CC=CC=C3NC(=O)C4=CC(Cl)=CC(Cl)=C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.4 (M + H)	3.55
3070	 <chem>CC1=NC2=CC=CC=C2N(C)N1C3=CC=CC=C3NC(=O)C4=CC(OC)=CC(OC)=C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	3.63

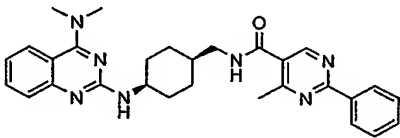
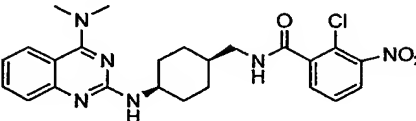
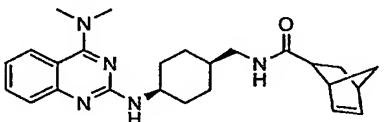
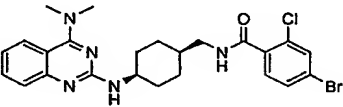
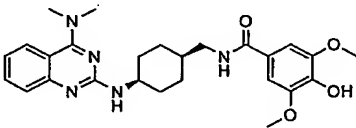
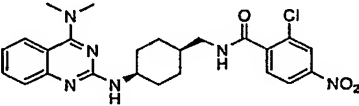
Example No.	Structure	ESI-MS	Retention Time (min)
3071	 CF ₃ CO ₂ H	458.2 (M + H)	3.69
3072	 CF ₃ CO ₂ H	440.4 (M + H)	3.69
3073	 CF ₃ CO ₂ H	440.4 (M + H)	3.66
3074	 CF ₃ CO ₂ H	422.4 (M + H)	3.55
3075	 CF ₃ CO ₂ H	460.4 (M + H)	4.24
3076	 CF ₃ CO ₂ H	429.2 (M + H)	3.42

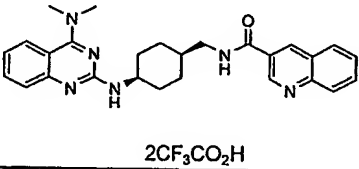
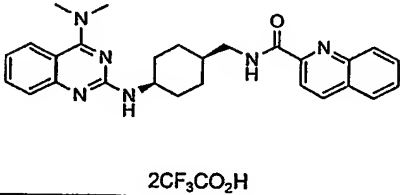
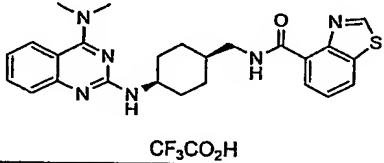
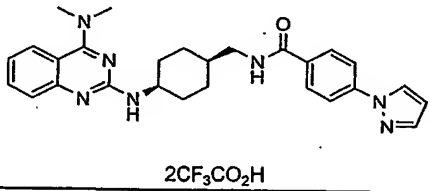
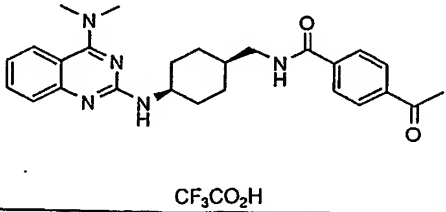
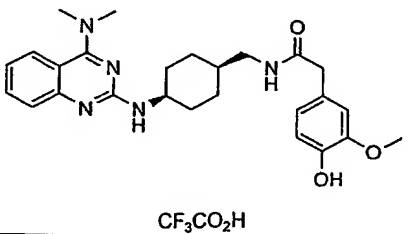
Example No.	Structure	ESI-MS	Retention Time (min)
3077	 <chem>COc1ccc(cc1)C(=O)NCC2CCCCC2Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	3.61
3078	 <chem>COc1ccc(cc1)C(=O)NCC2CCCCC2Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	488.4 (M + H)	3.86
3079	 <chem>CCCCCOc1ccc(cc1)C(=O)NCC2CCCCC2Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	518.6 (M + H)	4.74
3080	 <chem>Fc1cc(F)c(F)cc1C(=O)NCC2CCCCC2Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	3.68
3081	 <chem>C1CCCCC1C(=O)NCC2CCCCC2Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	410.4 (M + H)	3.58
3082	 <chem>Cc1cc(C(F)(F)F)cc(C(F)(F)F)c1C(=O)NCC2CCCCC2Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	540.4 (M + H)	4.19

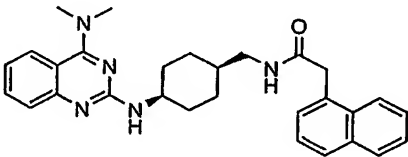
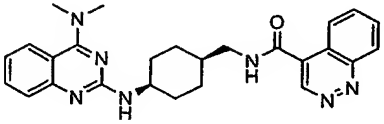
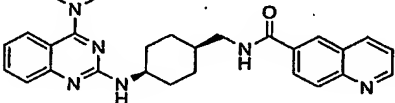
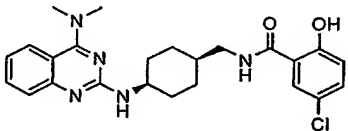
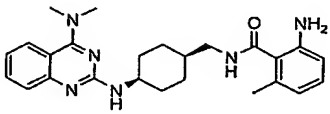
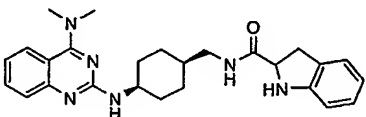
Example No.	Structure	ESI-MS	Retention Time (min)
3083	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC3CCCCC3C(=O)Nc4ccc(F)cc4)C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	422.2 (M + H)	3.50
3084	 <chem>COc1cc(OC)c(OC)c(C(=O)Nc2c3ccccc3n1n2)cc3CCCCC3C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	494.4 (M + H)	3.39
3085	 <chem>FC1=CC=C(C(=O)Nc2c3ccccc3n1n2)C(F)=CC3</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.0 (M + H)	3.55
3086	 <chem>Clc1ccccc1C(=O)Nc2c3ccccc3n1n2C4CCCCC4C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	438.2 (M + H)	3.48
3087	 <chem>c1ccc2ccccc2c1C(=O)Nc3c4ccccc4n1n3C5CCCCC5C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	454.2 (M + H)	3.75
3088	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC3CCCCC3C(=O)Nc4ccc(C(F)(F)F)cc4)C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.4 (M + H)	3.83

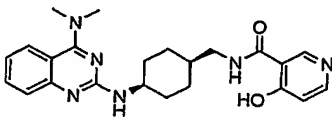
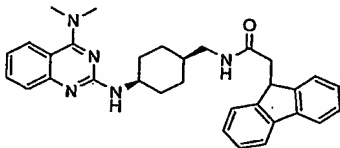
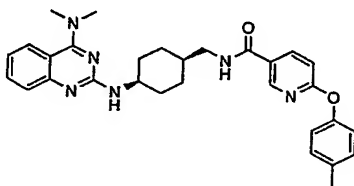
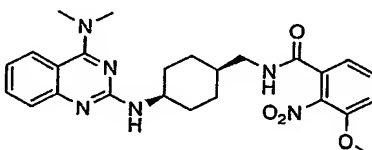
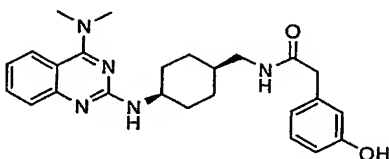
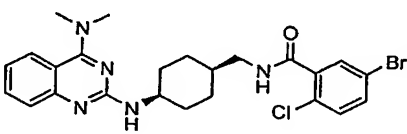
Example No.	Structure	ESI-MS	Retention Time (min)
3089	 <chem>CC1=NC2=CC=CC=C2N(C)N=C1N[C@H]3CCCC[C@H]3NC(=O)c4ccc(F)cc4</chem> <chem>CC(F)(F)C(=O)O</chem>	422.2 (M + H)	3.51
3090	 <chem>CC1=NC2=CC=CC=C2N(C)N=C1N[C@H]3CCCC[C@H]3NC(=O)c4ccc(C(F)(F)F)cc4</chem> <chem>CC(F)(F)C(=O)O</chem>	472.4 (M + H)	3.87
3091	 <chem>CC1=NC2=CC=CC=C2N(C)N=C1N[C@H]3CCCC[C@H]3NC(=O)c4cc(F)cc(Br)c4</chem> <chem>CC(F)(F)C(=O)O</chem>	500.4 (M + H)	3.03
3092	 <chem>CC1=NC2=CC=CC=C2N(C)N=C1N[C@H]3CCCC[C@H]3NC(=O)c4ccc(N(C)C)cc4</chem> <chem>CC(F)(F)C(=O)O</chem>	447.4 (M + H)	2.59
3093	 <chem>CC1=NC2=CC=CC=C2N(C)N=C1N[C@H]3CCCC[C@H]3NC(=O)c4ccc(C1=CC=CC=C1S)cc4</chem> <chem>CC(F)(F)C(=O)O</chem>	486.4 (M + H)	3.25
3094	 <chem>CC1=NC2=CC=CC=C2N(C)N=C1N[C@H]3CCCC[C@H]3NC(=O)c4ccc(C1=NC=NC=N1)cc4</chem> <chem>CC(F)(F)C(=O)O</chem>	488.4 (M + H)	2.81

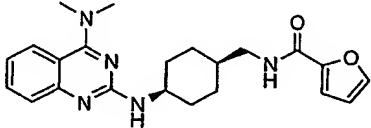
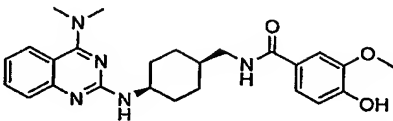
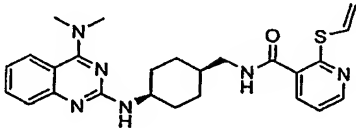
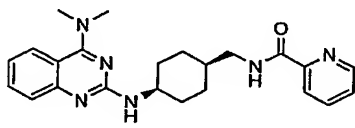
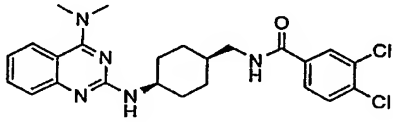
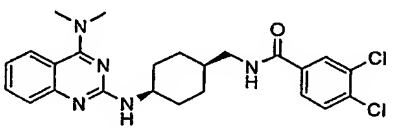
Example No.	Structure	ESI-MS	Retention Time (min)
3095	 <chem>CC1=CC=C(C=C1)N2C(=NC3=CC=CC=C3N(C)C=C2N)C4CCCCC4CCNC(=O)C1=CC=C(C=C1)C</chem> $\text{CF}_3\text{CO}_2\text{H}$	452.4 (M + H)	2.98
3096	 <chem>CC1=CC=C(C=C1)N2C(=NC3=CC=CC=C3N(C)C=C2N)C4CCCCC4CCNC(=O)C1=CC=C(C=C1)OC2=CC=CC=C2</chem> $\text{CF}_3\text{CO}_2\text{H}$	496.4 (M + H)	3.29
3097	 <chem>CC1=CC=C(C=C1)N2C(=NC3=CC=CC=C3N(C)C=C2N)C4CCCCC4CCNC(=O)C1(C)C=CC=C1OC</chem> $\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	2.77
3098	 <chem>CC1=CC=C(C=C1)N2C(=NC3=CC=CC=C3N(C)C=C2N)C4CCCCC4CCNC(=O)C1=CC2=CC=CC=C2C3=CC=CC=C13</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.4 (M + H)	3.06
3099	 <chem>CC1=CC=C(C=C1)N2C(=NC3=CC=CC=C3N(C)C=C2N)C4CCCCC4CCNC(=O)C1=C(C)OC=C1C2=CC=CC=C2</chem> $\text{CF}_3\text{CO}_2\text{H}$	484.4 (M + H)	3.40
3100	 <chem>CC1=CC=C(C=C1)N2C(=NC3=CC=CC=C3N(C)C=C2N)C4CCCCC4CCNC(=O)CC1=CC=CC=C1</chem> $\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	2.69

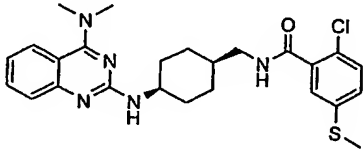
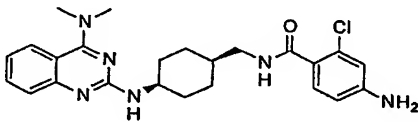
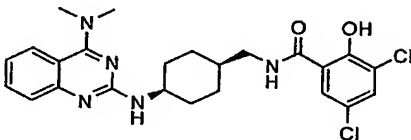
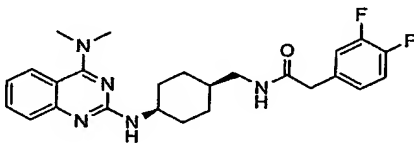
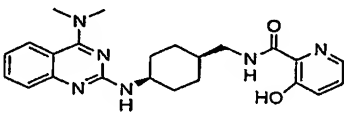
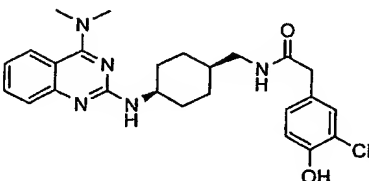
Example No.	Structure	ESI-MS	Retention Time (min)
3101	 <chem>CC1=CN(C)C2=CC=CC=C2N1C3=CC=CC=C3C(=O)NCC4CCCCC4N5C(=O)C6=CC=CC=C6C5=N4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	496.4 (M + H)	3.01
3102	 <chem>CC1=CN(C)C2=CC=CC=C2N1C3=CC=CC=C3C(=O)NCC4CCCCC4N5C(=O)C6=CC(=CC=C6)C(=O)N5</chem> $\text{CF}_3\text{CO}_2\text{H}$	483.4 (M + H)	2.79
3103	 <chem>CC1=CN(C)C2=CC=CC=C2N1C3=CC=CC=C3C(=O)NCC4CCCCC4N5C(=O)C6=CC=CC=C6C5=N4</chem> $\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.76
3104	 <chem>CC1=CN(C)C2=CC=CC=C2N1C3=CC=CC=C3C(=O)NCC4CCCCC4N5C(=O)C6=CC(=CC=C6)C(=O)N5</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.2 (M + H)	3.03
3105	 <chem>CC1=CN(C)C2=CC=CC=C2N1C3=CC=CC=C3C(=O)NCC4CCCCC4N5C(=O)C6=CC(=CC=C6)C(=O)N5</chem> $\text{CF}_3\text{CO}_2\text{H}$	480.4 (M + H)	2.41
3106	 <chem>CC1=CN(C)C2=CC=CC=C2N1C3=CC=CC=C3C(=O)NCC4CCCCC4N5C(=O)C6=CC(=CC=C6)C(=O)N5</chem> $\text{CF}_3\text{CO}_2\text{H}$	483.2 (M + H)	2.84

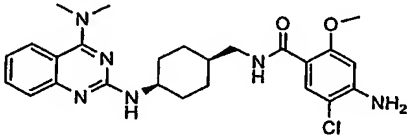
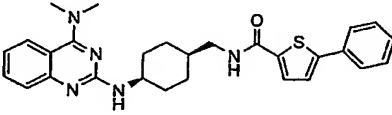
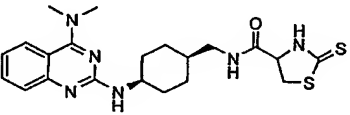
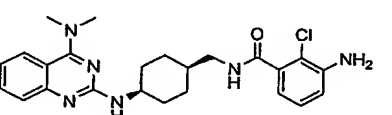
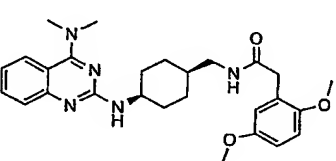
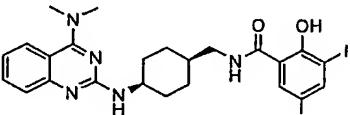
Example No.	Structure	ESI-MS	Retention Time (min)
3107	 2CF ₃ CO ₂ H	455 (M + H)	2.45
3108	 2CF ₃ CO ₂ H	455.2 (M + H)	3.19
3109	 CF ₃ CO ₂ H	461.4 (M + H)	2.60
3110	 2CF ₃ CO ₂ H	470.4 (M + H)	2.74
3111	 CF ₃ CO ₂ H	446.6 (M + H)	2.61
3112	 CF ₃ CO ₂ H	464.4 (M + H)	2.35

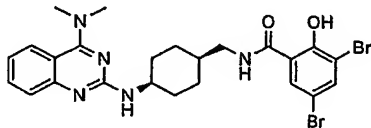
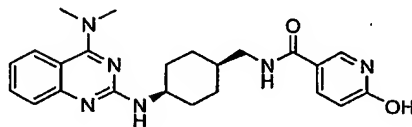
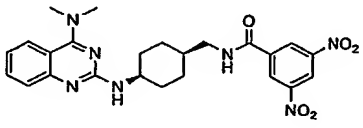
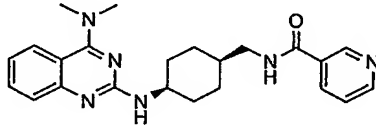
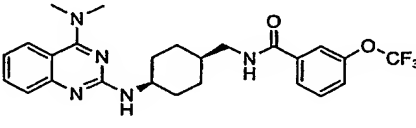
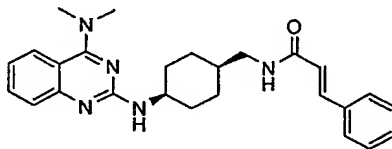
Example No.	Structure	ESI-MS	Retention Time (min)
3113	 <chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC(=C3)N(C)C)C4CCCCC4CC(=O)NCC5=CC=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	468.4 (M + H)	3.04
3114	 $2\text{CF}_3\text{CO}_2\text{H}$	456.2 (M + H)	2.44
3115	 $2\text{CF}_3\text{CO}_2\text{H}$	455.2 (M + H)	2.11
3116	 $\text{CF}_3\text{CO}_2\text{H}$	454.2 (M + H)	3.21
3117	 $2\text{CF}_3\text{CO}_2\text{H}$	433.6 (M + H)	2.34
3118	 $2\text{CF}_3\text{CO}_2\text{H}$	444.6 (M+)	2.93

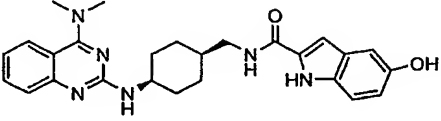
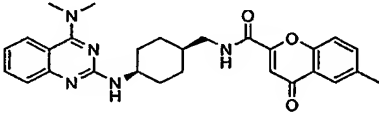
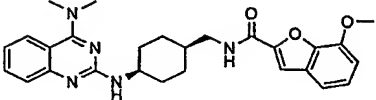
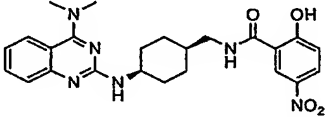
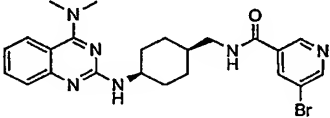
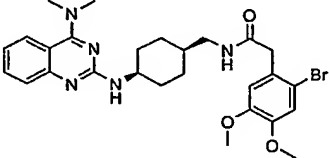
Example No.	Structure	ESI-MS	Retention Time (min)
3119	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3CCNC(=O)C4=CC=CC=C4O</chem> $2\text{CF}_3\text{CO}_2\text{H}$	421.4 (M + H)	2.23
3120	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3CCNC(=O)CC4=CC5=CC=CC=C5C6=CC=CC=C46</chem> $\text{CF}_3\text{CO}_2\text{H}$	506.4 (M + H)	3.31
3121	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3CCNC(=O)c4cc(Oc5ccc(OC)cc5)ncn4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	511.6 (M + H)	3.21
3122	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3CCNC(=O)C4=CC(OC)=CC(=C4)[N+](=O)[O-]</chem> $\text{CF}_3\text{CO}_2\text{H}$	479.4 (M + H)	3.60
3123	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3CCNC(=O)CC4=CC=CC=C4O</chem> $\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	2.37
3124	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3CCNC(=O)C4=CC(=CC=C4Cl)C(=O)C5=CC=CC=C5Br</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.4 (M + H)	3.02

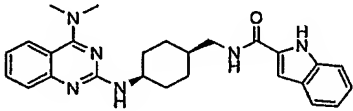
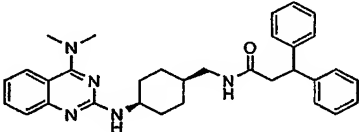
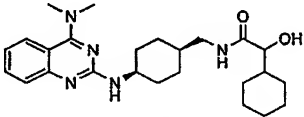
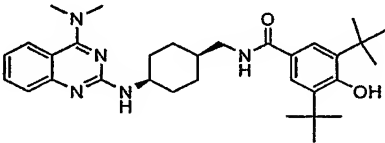
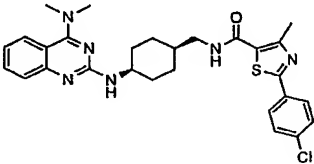
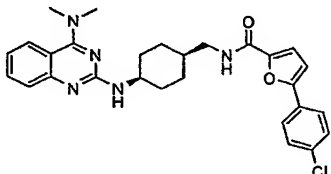
Example No.	Structure	ESI-MS	Retention Time (min)
3125	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CN(C(=O)C4=CC=CO4)</chem> $\text{CF}_3\text{CO}_2\text{H}$	394.4 (M + H)	2.45
3126	 <chem>COc1cccc(c1)C(=O)N[C@H]2CCCC[C@H]2N[C@@H]3C4=CC=CC=C4N(C)N3</chem> $\text{CF}_3\text{CO}_2\text{H}$	450.2 (M + H)	2.41
3127	 <chem>C=CSc1cccc(c1)C(=O)N[C@H]2CCCC[C@H]2N[C@@H]3C4=CC=CC=C4N(C)N3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	477.0 (M + H)	2.88
3128	 <chem>c1ccncc1C(=O)N[C@H]2CCCC[C@H]2N[C@@H]3C4=CC=CC=C4N(C)N3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	405.6 (M + H)	2.61
3129	 <chem>Clc1cc(Cl)ccc1C(=O)N[C@H]2CCCC[C@H]2N[C@@H]3C4=CC=CC=C4N(C)N3</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.6 (M + H)	3.17
3130	 <chem>Clc1cc(Cl)ccc1C(=O)N[C@H]2CCCC[C@H]2N[C@@H]3C4=CC=CC=C4N(C)N3</chem> $\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	2.59

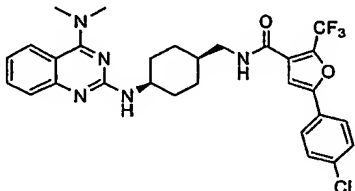
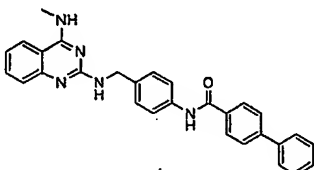
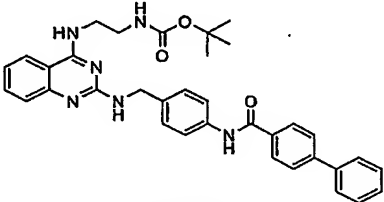
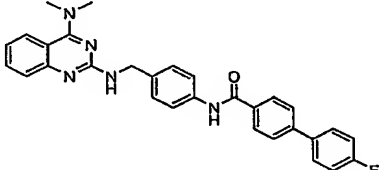
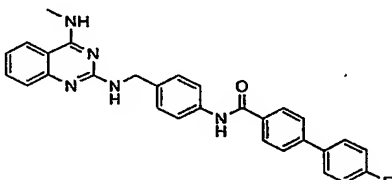
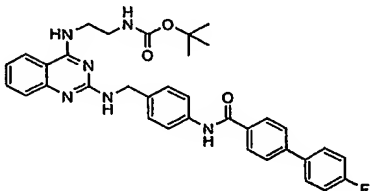
Example No.	Structure	ESI-MS	Retention Time (min)
3131	 $\text{CF}_3\text{CO}_2\text{H}$	484.2 (M + H)	2.99
3132	 $2\text{CF}_3\text{CO}_2\text{H}$	453.0 (M + H)	2.45
3133	 $\text{CF}_3\text{CO}_2\text{H}$	488.4 (M + H)	3.59
3134	 $\text{CF}_3\text{CO}_2\text{H}$	454.2 (M + H)	2.81
3135	 $2\text{CF}_3\text{CO}_2\text{H}$	421.4 (M + H)	2.89
3136	 $\text{CF}_3\text{CO}_2\text{H}$	468.4 (M + H)	2.53

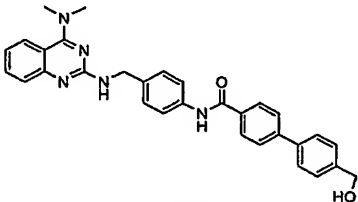
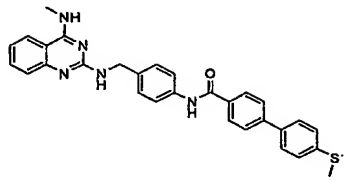
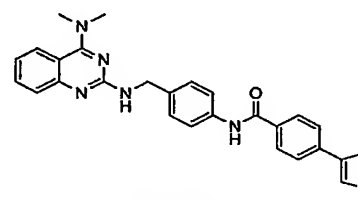
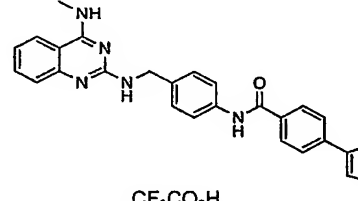
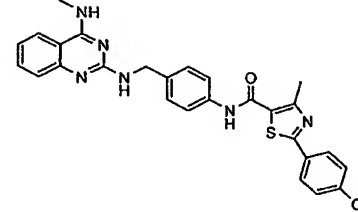
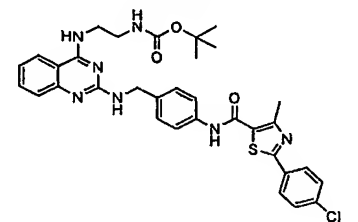
Example No.	Structure	ESI-MS	Retention Time (min)
3137	 <chem>CN(C)c1nc(NC2CCCCC2CNC(=O)c3cc(OC)c(N)c(Cl)c3)c4ccccc14</chem> $2\text{CF}_3\text{CO}_2\text{H}$	483.2 (M + H)	2.83
3138	 <chem>CN(C)c1nc(NC2CCCCC2CNC(=O)c3cc(C4=CC=CC=C4)s3)c4ccccc14</chem> $\text{CF}_3\text{CO}_2\text{H}$	487.4 (M+2H+)	3.40
3139	 <chem>CN(C)c1nc(NC2CCCCC2CNC(=O)N3CCSC3)c4ccccc14</chem> $\text{CF}_3\text{CO}_2\text{H}$	445.6 (M + H)	2.36
3140	 <chem>Nc1cc(NC2CCCCC2CNC(=O)c3cc(N)ccc3Cl)c4ccccc14</chem> $2\text{CF}_3\text{CO}_2\text{H}$	453.2 (M + H)	2.46
3141	 <chem>COC1=CC(OC)=CC(OC)=C1C(=O)NC2CCCCC2CNC3=C4C=CC=CC=C4N(C)N3</chem> $\text{CF}_3\text{CO}_2\text{H}$	478.4 (M + H)	2.77
3142	 <chem>Oc1cc(I)cc(I)c1C(=O)NC2CCCCC2CNC3=C4C=CC=CC=C4N(C)N3</chem> $\text{CF}_3\text{CO}_2\text{H}$	672.2 (M + H)	3.92

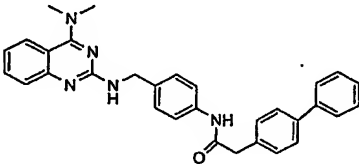
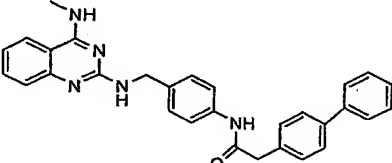
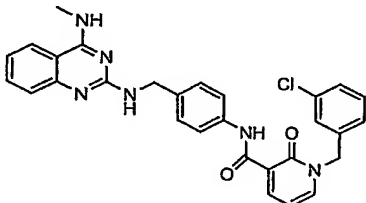
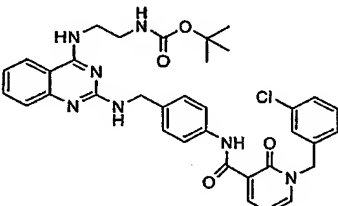
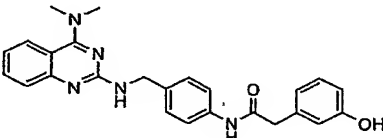
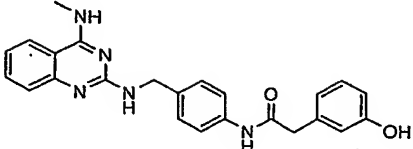
Example No.	Structure	ESI-MS	Retention Time (min)
3143	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNC(=O)c1cc(Br)cc(Br)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	576.2 (M + H)	3.71
3144	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNC(=O)c1ccncc1O</chem> $2\text{CF}_3\text{CO}_2\text{H}$	421.2 (M + H)	2.01
3145	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	494.4 (M + H)	2.77
3146	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNC(=O)c1ccncc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	405.6 (M + H)	1.99
3147	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNC(=O)c1ccc(OC(F)(F)F)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	488.4 (M + H)	3.13
3148	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNC(=O)C=Cc1ccccc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	430.4 (M + H)	2.91

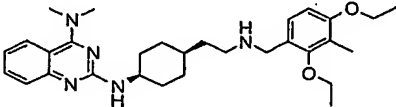
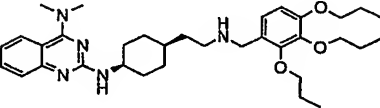
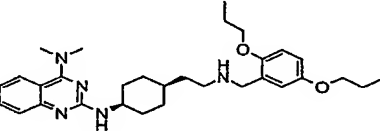
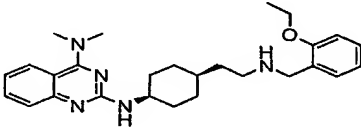
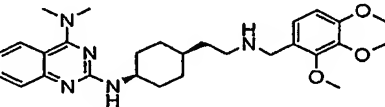
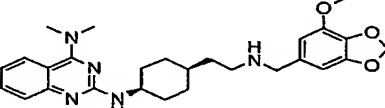
Example No.	Structure	ESI-MS	Retention Time (min)
3149	 <chem>CN(C)c1nc2c(ncn2C1)C(=O)NCC3CCCCC3NC(=O)c4c[nH]c5ccc(O)cc45</chem> $2\text{CF}_3\text{CO}_2\text{H}$	459.4 (M + H)	2.47
3150	 <chem>CN(C)c1nc2c(ncn2C1)C(=O)NCC3CCCCC3NC(=O)c4cc5c(c(=O)oc45)C</chem> $\text{CF}_3\text{CO}_2\text{H}$	486.6 (M + H)	2.93
3151	 <chem>CN(C)c1nc2c(ncn2C1)C(=O)NCC3CCCCC3NC(=O)c4cc5c(c(=O)oc45)OC</chem> $\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	3.03
3152	 <chem>CN(C)c1nc2c(ncn2C1)C(=O)NCC3CCCCC3NC(=O)c4cc(O)cc([N+](=O)[O-])c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	465.2 (M + H)	3.13
3153	 <chem>CN(C)c1nc2c(ncn2C1)C(=O)NCC3CCCCC3NC(=O)c4ccncc4Br</chem> $2\text{CF}_3\text{CO}_2\text{H}$	483.4 (M + H)	2.67
3154	 <chem>CN(C)c1nc2c(ncn2C1)C(=O)NCC3CCCCC3NC(=O)Cc4cc(OC)c(OC)c4Br</chem> $\text{CF}_3\text{CO}_2\text{H}$	556.4 (M + H)	2.84

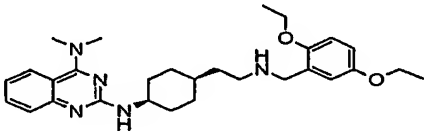
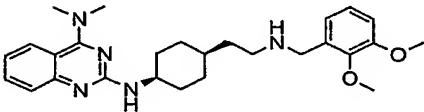
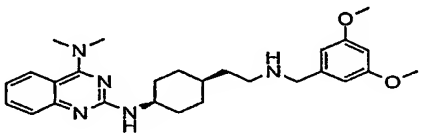
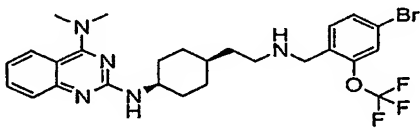
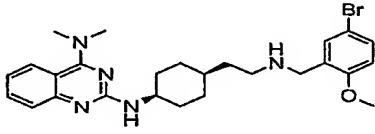
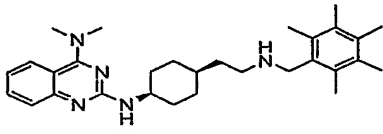
Example No.	Structure	ESI-MS	Retention Time (min)
3155	 <chem>CC1=NC2=CC=CC=C2N(C)=NC1NCC3CCCCC3NC(=O)c4c[nH]c5ccccc45</chem> $2\text{CF}_3\text{CO}_2\text{H}$	443.4 (M + H)	2.94
3156	 <chem>CC1=NC2=CC=CC=C2N(C)=NC1NCC3CCCCC3NC(=O)Cc4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	508.2 (M + H)	3.20
3157	 <chem>CC1=NC2=CC=CC=C2N(C)=NC1NCC3CCCCC3NC(=O)C4CCCCC4O</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.0 (M + H)	2.72
3158	 <chem>CC1=NC2=CC=CC=C2N(C)=NC1NCC3CCCCC3NC(=O)c4c(O)c(C)(C)cc(C)(C)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	532.4 (M + H)	3.58
3159	 <chem>CC1=NC2=CC=CC=C2N(C)=NC1NCC3CCCCC3NC(=O)c4cc(Cl)ccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	535.4 (M + H)	3.51
3160	 <chem>CC1=NC2=CC=CC=C2N(C)=NC1NCC3CCCCC3NC(=O)c4ccc(Cl)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	504.4 (M + H)	3.49

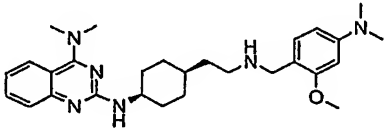
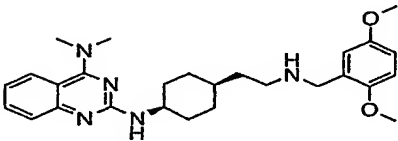
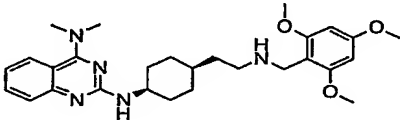
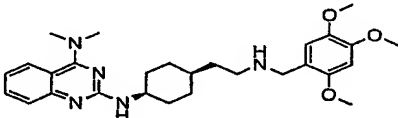
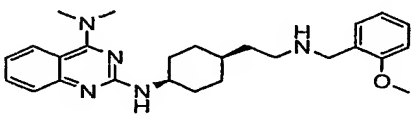
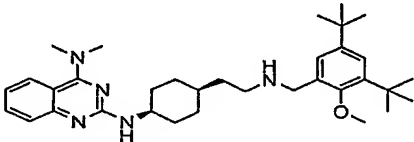
Example No.	Structure	ESI-MS	Retention Time (min)
3161	 <chem>CC1=NC2=CC=CC=C2N1CNC3CCCCC3NC(=O)c4oc(cc4C(F)(F)F)c5ccc(Cl)cc5</chem> <chem>CF3CO2H</chem>	572.4 (M + H)	3.71
3162	 <chem>Nc1nc2ccccc2n1CNc3ccc(NC(=O)c4ccc(cc4)cc5ccccc5)cc3</chem> <chem>CF3CO2H</chem>	460.2 (M + H)	3.80
3163	 <chem>CC(C)(C)OC(=O)NCCNc1nc2ccccc2n1CNc3ccc(NC(=O)c4ccc(cc4)cc5ccccc5)cc3</chem> <chem>CF3CO2H</chem>	589.2 (M + H)	4.00
3164	 <chem>Nc1nc2ccccc2n1CNc3ccc(NC(=O)c4ccc(cc4)cc5ccc(F)cc5)cc3</chem> <chem>CF3CO2H</chem>	492.2 (M + H)	3.90
3165	 <chem>CNc1nc2ccccc2n1CNc3ccc(NC(=O)c4ccc(cc4)cc5ccc(F)cc5)cc3</chem> <chem>CF3CO2H</chem>	478.2 (M + H)	3.80
3166	 <chem>CC(C)(C)OC(=O)NCCNc1nc2ccccc2n1CNc3ccc(NC(=O)c4ccc(cc4)cc5ccc(F)cc5)cc3</chem> <chem>CF3CO2H</chem>	607.6 (M + H)	4.00

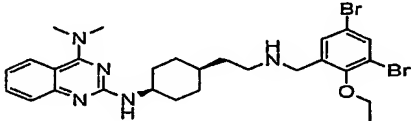
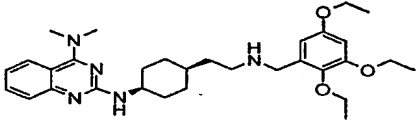
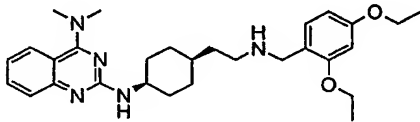
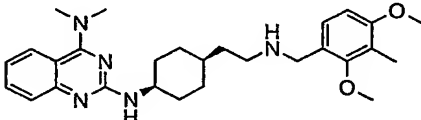
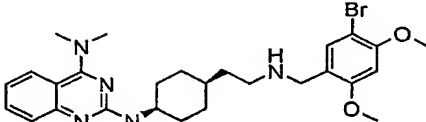
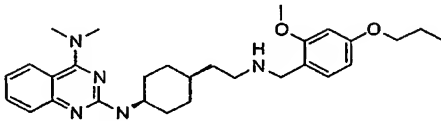
Example No.	Structure	ESI-MS	Retention Time (min)
3167	 <chem>CC1=NC=NC(NC1Cc2ccc(NC(=O)c3ccc(O)cc3)cc2)c4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	504.2 (M + H)	3.40
3168	 <chem>CC1=NC=NC(NC1Cc2ccc(NC(=O)c3ccc(SC)cc3)cc2)c4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	506.2 (M + H)	3.90
3169	 <chem>CC1=NC=NC(NC1Cc2ccc(NC(=O)c3ccc(C4=CC=CS4)cc3)cc2)c4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	480.2 (M + H)	3.80
3170	 <chem>CC1=NC=NC(NC1Cc2ccc(NC(=O)c3ccc(C4=CC=CS4)cc3)cc2)c4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	466.2 (M + H)	3.70
3171	 <chem>CC1=NC=NC(NC1Cc2ccc(NC(=O)c3c(C4=CC=CC=C4)nn(C4=CC=CC=C4)s3)cc2)c4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	515.2 (M + H)	3.90
3172	 <chem>CC1=NC=NC(NC1Cc2ccc(NC(=O)c3c(C4=CC=CC=C4)nn(C4=CC=CC=C4)s3)cc2)c4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	644.2 (M + H)	4.10

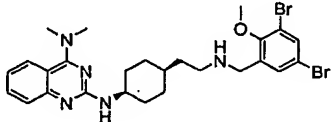
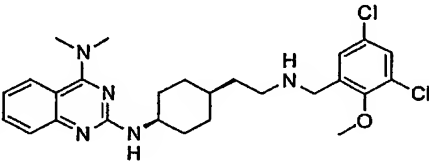
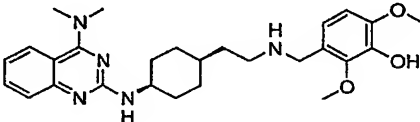
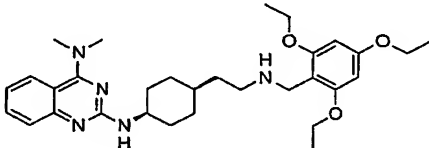
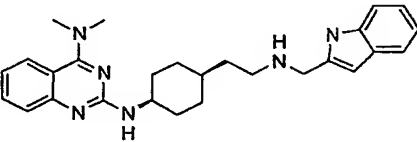
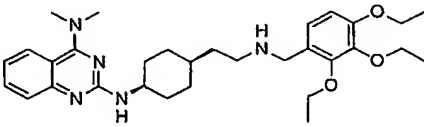
Example No.	Structure	ESI-MS	Retention Time (min)
3173	 <chem>CC1=NC2=C(N1)N=CN=C2CNc3ccc(NC(=O)Cc4ccc(cc4)-c5ccccc5)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	488.2 (M + H)	3.90
3174	 <chem>Nc1nc2ccccc2n1CNc3ccc(NC(=O)Cc4ccc(cc4)-c5ccccc5)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	3.80
3175	 <chem>Nc1nc2ccccc2n1CNc3ccc(NC(=O)c4cc(Cl)ccc4Cc5ccccc5n5c6ccccc6c5=O)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	525.4 (M + H)	3.70
3176	 <chem>CC(C)(C)OC(=O)NCCNc1nc2ccccc2n1CNc3ccc(NC(=O)c4cc(Cl)ccc4Cc5ccccc5n5c6ccccc6c5=O)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	654.2 (M + H)	3.90
3177	 <chem>CC1=NC2=C(N1)N=CN=C2CNc3ccc(NC(=O)Cc4ccc(O)cc4)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	428.2 (M + H)	3.10
3178	 <chem>Nc1nc2ccccc2n1CNc3ccc(NC(=O)Cc4ccc(O)cc4)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	414.4 (M + H)	2.90

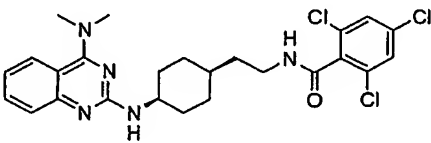
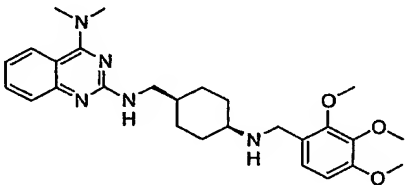
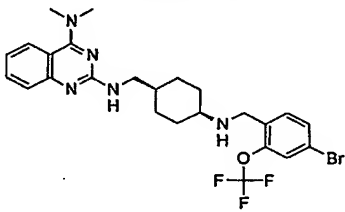
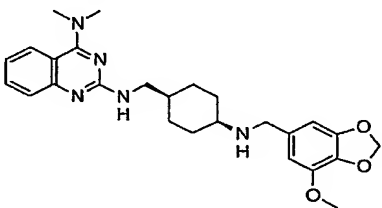
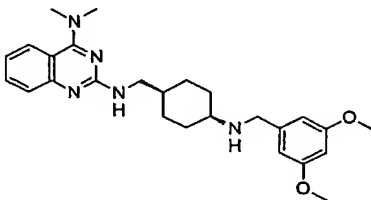
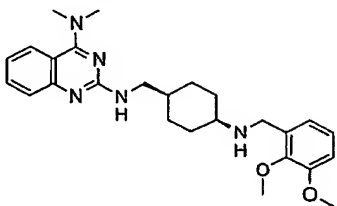
Example No.	Structure	ESI-MS	Retention Time (min)
3179	 <chem>CCOC1=CC=C(C=C1C)NCNCC2(CCC2)NCC3=NC4=CC=CC=C4N(C)N3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	506.4 (M + H)	3.04
3180	 <chem>CCOC1=CC(=CC(=C1)OCC)NCNCC2(CCC2)NCC3=NC4=CC=CC=C4N(C)N3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	578.8 (M + H)	3.50
3181	 <chem>CCOC1=CC(=CC(=C1)OCC)NCNCC2(CCC2)NCC3=NC4=CC=CC=C4N(C)N3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	520.6 (M + H)	3.19
3182	 <chem>CCOC1=CC(=CC(=C1)OCC)NCNCC2(CCC2)NCC3=NC4=CC=CC=C4N(C)N3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	2.80
3183	 <chem>CCOC1=CC(=CC(=C1)OCC)NCNCC2(CCC2)NCC3=NC4=CC=CC=C4N(C)N3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	494.6 (M + H)	2.66
3184	 <chem>CCOC1=CC(=CC(=C1)OCC)NCNCC2(CCC2)NCC3=NC4=CC=CC=C4N(C)N3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	478.4 (M + H)	2.66

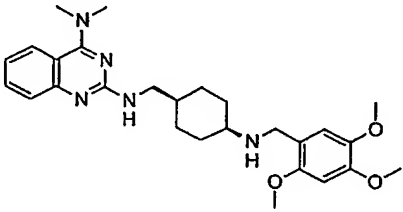
Example No.	Structure	ESI-MS	Retention Time (min)
3185	 $2\text{CF}_3\text{CO}_2\text{H}$	492.6 (M + H)	2.94
3186	 $2\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	2.65
3187	 $2\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	2.68
3188	 $2\text{CF}_3\text{CO}_2\text{H}$	566.4 (M + H)	3.03
3189	 $2\text{CF}_3\text{CO}_2\text{H}$	512.6 (M + H)	2.85
3190	 $2\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	3.09

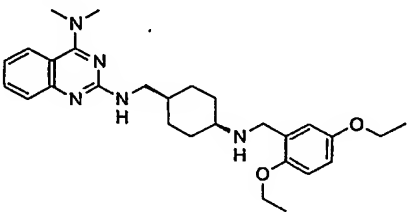
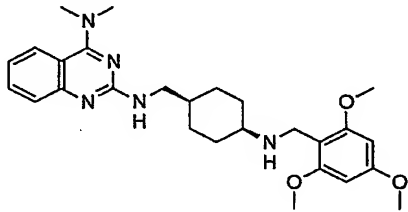
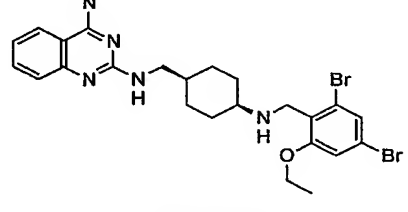
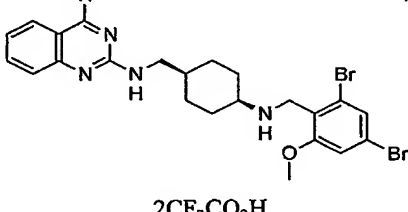
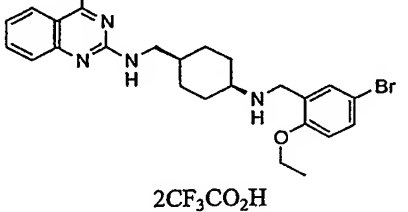
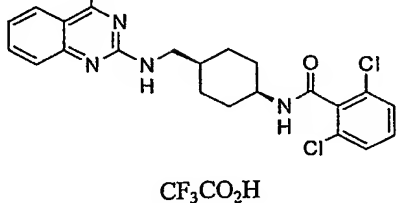
Example No.	Structure	ESI-MS	Retention Time (min)
3191	 $3\text{CF}_3\text{CO}_2\text{H}$	477.4 (M + H)	2.51
3192	 $2\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	2.67
3193	 $2\text{CF}_3\text{CO}_2\text{H}$	494.6 (M + H)	2.78
3194	 $2\text{CF}_3\text{CO}_2\text{H}$	494.6 (M + H)	2.60
3195	 $2\text{CF}_3\text{CO}_2\text{H}$	434.6 (M + H)	2.67
3196	 $2\text{CF}_3\text{CO}_2\text{H}$	546.4 (M + H)	4.30

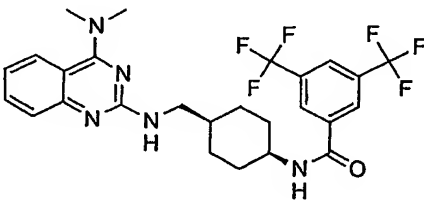
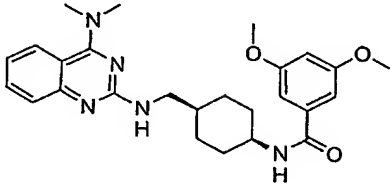
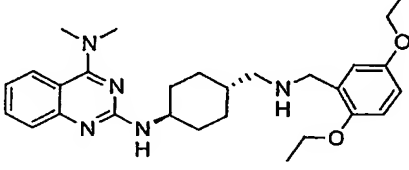
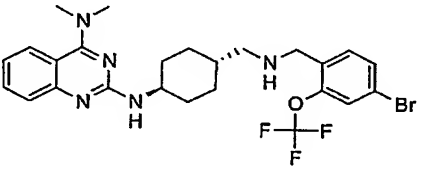
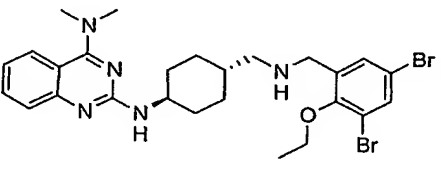
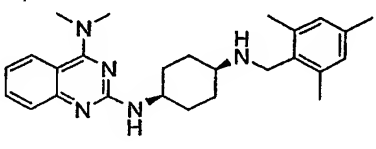
Example No.	Structure	ESI-MS	Retention Time (min)
3197	 <chem>CN(C)c1nc2c(nc3ccccc13)nc(NCC4CCCCC4CCNCC5=CC(=C(C=C5)Br)BrOCC)cc2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	606.6 (M + H)	3.95
3198	 <chem>CN(C)c1nc2c(nc3ccccc13)nc(NCC4CCCCC4CCNCC5=CC(=C(C=C5)OCC)OCC)cc2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	536.6 (M + H)	3.83
3199	 <chem>CN(C)c1nc2c(nc3ccccc13)nc(NCC4CCCCC4CCNCC5=CC(=CC=C5)OCC)cc2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	492.4 (M + H)	2.97
3200	 <chem>CN(C)c1nc2c(nc3ccccc13)nc(NCC4CCCCC4CCNCC5=CC(=C(C=C5)OC)OC)cc2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	478.4 (M + H)	2.79
3201	 <chem>CN(C)c1nc2c(nc3ccccc13)nc(NCC4CCCCC4CCNCC5=CC(=C(C=C5)Br)OC)cc2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	542.0 (M + H)	2.85
3202	 <chem>CN(C)c1nc2c(nc3ccccc13)nc(NCC4CCCCC4CCNCC5=CC(=CC=C5)OCC)cc2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	492.6 (M + H)	2.81

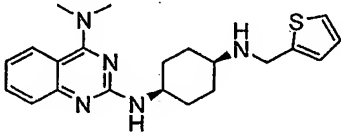
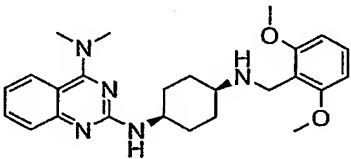
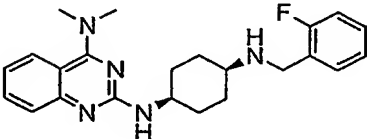
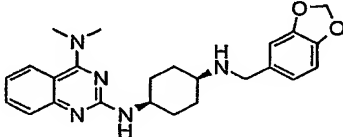
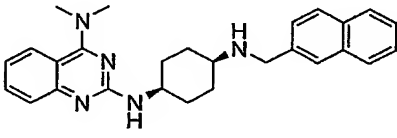
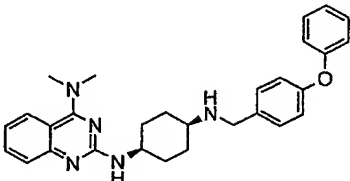
Example No.	Structure	ESI-MS	Retention Time (min)
3203	 $2\text{CF}_3\text{CO}_2\text{H}$	590.4 (M + H)	3.02
3204	 $2\text{CF}_3\text{CO}_2\text{H}$	502.2 (M + H)	2.91
3205	 $2\text{CF}_3\text{CO}_2\text{H}$	480.4 (M + H)	2.51
3206	 $2\text{CF}_3\text{CO}_2\text{H}$	536.4 (M + H)	3.21
3207	 $3\text{CF}_3\text{CO}_2\text{H}$	443.6 (M + H)	2.66
3208	 $2\text{CF}_3\text{CO}_2\text{H}$	536.4 (M + H)	3.08

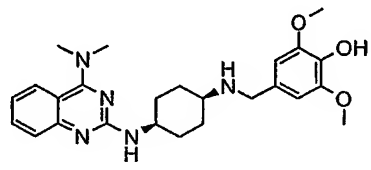
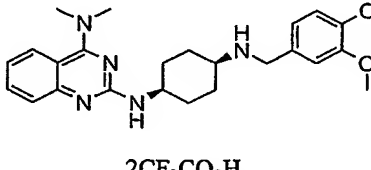
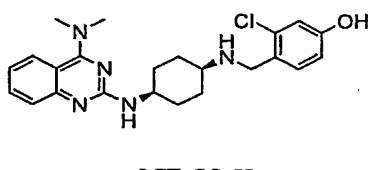
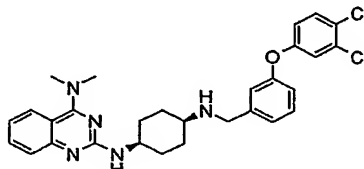
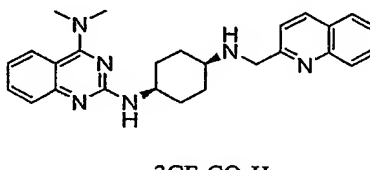
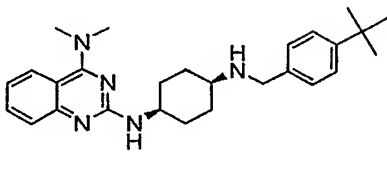
Example No.	Structure	ESI-MS	Retention Time (min)
3209	 $2\text{CF}_3\text{CO}_2\text{H}$	520.0 (M + H)	3.51
3210	 $2\text{CF}_3\text{CO}_2\text{H}$	480.4 (M + H)	2.58
3211	 $2\text{CF}_3\text{CO}_2\text{H}$	552.0 (M + H)	3.11
3212	 $2\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	3.22
3213	 $2\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	2.70
3214	 $2\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	2.58

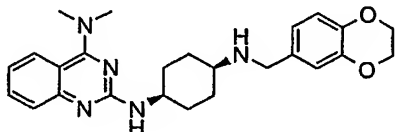
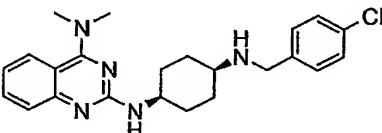
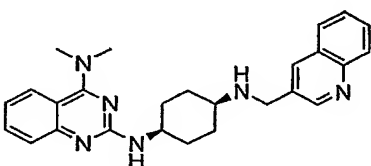
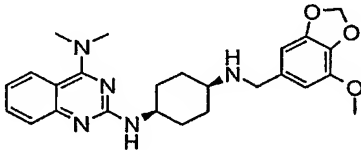
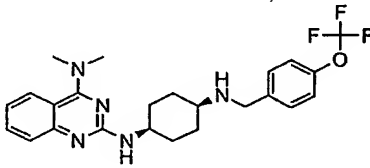
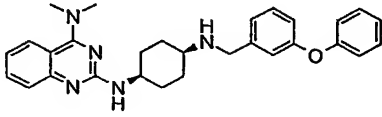
Example No.	Structure	ESI-MS	Retention Time (min)
3215	 <chem>COc1ccc(cc1)CN(Cc2ccccc2N(C)N)C3CCCCC3CN(Cc4ccc(OC)cc4)C5CCCCC5CN(Cc6ccc(OC)cc6)C7CCCCC7CN(Cc8ccc(OC)cc8)C9CCCCC9CN(Cc10ccc(OC)cc10)C11CCCCC11CN(Cc12ccc(OC)cc12)C13CCCCC13CN(Cc14ccc(OC)cc14)C15CCCCC15CN(Cc16ccc(OC)cc16)C17CCCCC17CN(Cc18ccc(OC)cc18)C19CCCCC19CN(Cc20ccc(OC)cc20)C21CCCCC21CN(Cc22ccc(OC)cc22)C23CCCCC23CN(Cc24ccc(OC)cc24)C25CCCCC25CN(Cc26ccc(OC)cc26)C27CCCCC27CN(Cc28ccc(OC)cc28)C29CCCCC29CN(Cc30ccc(OC)cc30)C31CCCCC31CN(Cc32ccc(OC)cc32)C33CCCCC33CN(Cc34ccc(OC)cc34)C35CCCCC35CN(Cc36ccc(OC)cc36)C37CCCCC37CN(Cc38ccc(OC)cc38)C39CCCCC39CN(Cc40ccc(OC)cc40)C41CCCCC41CN(Cc42ccc(OC)cc42)C43CCCCC43CN(Cc44ccc(OC)cc44)C45CCCCC45CN(Cc46ccc(OC)cc46)C47CCCCC47CN(Cc48ccc(OC)cc48)C49CCCCC49CN(Cc50ccc(OC)cc50)C51CCCCC51CN(Cc52ccc(OC)cc52)C53CCCCC53CN(Cc54ccc(OC)cc54)C55CCCCC55CN(Cc56ccc(OC)cc56)C57CCCCC57CN(Cc58ccc(OC)cc58)C59CCCCC59CN(Cc60ccc(OC)cc60)C61CCCCC61CN(Cc62ccc(OC)cc62)C63CCCCC63CN(Cc64ccc(OC)cc64)C65CCCCC65CN(Cc66ccc(OC)cc66)C67CCCCC67CN(Cc68ccc(OC)cc68)C69CCCCC69CN(Cc70ccc(OC)cc70)C71CCCCC71CN(Cc72ccc(OC)cc72)C73CCCCC73CN(Cc74ccc(OC)cc74)C75CCCCC75CN(Cc76ccc(OC)cc76)C77CCCCC77CN(Cc78ccc(OC)cc78)C79CCCCC79CN(Cc80ccc(OC)cc80)C81CCCCC81CN(Cc82ccc(OC)cc82)C83CCCCC83CN(Cc84ccc(OC)cc84)C85CCCCC85CN(Cc86ccc(OC)cc86)C87CCCCC87CN(Cc88ccc(OC)cc88)C89CCCCC89CN(Cc90ccc(OC)cc90)C91CCCCC91CN(Cc92ccc(OC)cc92)C93CCCCC93CN(Cc94ccc(OC)cc94)C95CCCCC95CN(Cc96ccc(OC)cc96)C97CCCCC97CN(Cc98ccc(OC)cc98)C99CCCCC99CN(Cc100ccc(OC)cc100)C101CCCCC101CN(Cc102ccc(OC)cc102)C103CCCCC103CN(Cc104ccc(OC)cc104)C105CCCCC105CN(Cc106ccc(OC)cc106)C107CCCCC107CN(Cc108ccc(OC)cc108)C109CCCCC109CN(Cc110ccc(OC)cc110)C111CCCCC111CN(Cc112ccc(OC)cc112)C113CCCCC113CN(Cc114ccc(OC)cc114)C115CCCCC115CN(Cc116ccc(OC)cc116)C117CCCCC117CN(Cc118ccc(OC)cc118)C119CCCCC119CN(Cc120ccc(OC)cc120)C121CCCCC121CN(Cc122ccc(OC)cc122)C123CCCCC123CN(Cc124ccc(OC)cc124)C125CCCCC125CN(Cc126ccc(OC)cc126)C127CCCCC127CN(Cc128ccc(OC)cc128)C129CCCCC129CN(Cc130ccc(OC)cc130)C131CCCCC131CN(Cc132ccc(OC)cc132)C133CCCCC133CN(Cc134ccc(OC)cc134)C135CCCCC135CN(Cc136ccc(OC)cc136)C137CCCCC137CN(Cc138ccc(OC)cc138)C139CCCCC139CN(Cc140ccc(OC)cc140)C141CCCCC141CN(Cc142ccc(OC)cc142)C143CCCCC143CN(Cc144ccc(OC)cc144)C145CCCCC145CN(Cc146ccc(OC)cc146)C147CCCCC147CN(Cc148ccc(OC)cc148)C149CCCCC149CN(Cc150ccc(OC)cc150)C151CCCCC151CN(Cc152ccc(OC)cc152)C153CCCCC153CN(Cc154ccc(OC)cc154)C155CCCCC155CN(Cc156ccc(OC)cc156)C157CCCCC157CN(Cc158ccc(OC)cc158)C159CCCCC159CN(Cc160ccc(OC)cc160)C161CCCCC161CN(Cc162ccc(OC)cc162)C163CCCCC163CN(Cc164ccc(OC)cc164)C165CCCCC165CN(Cc166ccc(OC)cc166)C167CCCCC167CN(Cc168ccc(OC)cc168)C169CCCCC169CN(Cc170ccc(OC)cc170)C171CCCCC171CN(Cc172ccc(OC)cc172)C173CCCCC173CN(Cc174ccc(OC)cc174)C175CCCCC175CN(Cc176ccc(OC)cc176)C177CCCCC177CN(Cc178ccc(OC)cc178)C179CCCCC179CN(Cc180ccc(OC)cc180)C181CCCCC181CN(Cc182ccc(OC)cc182)C183CCCCC183CN(Cc184ccc(OC)cc184)C185CCCCC185CN(Cc186ccc(OC)cc186)C187CCCCC187CN(Cc188ccc(OC)cc188)C189CCCCC189CN(Cc190ccc(OC)cc190)C191CCCCC191CN(Cc192ccc(OC)cc192)C193CCCCC193CN(Cc194ccc(OC)cc194)C195CCCCC195CN(Cc196ccc(OC)cc196)C197CCCCC197CN(Cc198ccc(OC)cc198)C199CCCCC199CN(Cc200ccc(OC)cc200)C201CCCCC201CN(Cc202ccc(OC)cc202)C203CCCCC203CN(Cc204ccc(OC)cc204)C205CCCCC205CN(Cc206ccc(OC)cc206)C207CCCCC207CN(Cc208ccc(OC)cc208)C209CCCCC209CN(Cc210ccc(OC)cc210)C211CCCCC211CN(Cc212ccc(OC)cc212)C213CCCCC213CN(Cc214ccc(OC)cc214)C215CCCCC215CN(Cc216ccc(OC)cc216)C217CCCCC217CN(Cc218ccc(OC)cc218)C219CCCCC219CN(Cc220ccc(OC)cc220)C221CCCCC221CN(Cc222ccc(OC)cc222)C223CCCCC223CN(Cc224ccc(OC)cc224)C225CCCCC225CN(Cc226ccc(OC)cc226)C227CCCCC227CN(Cc228ccc(OC)cc228)C229CCCCC229CN(Cc230ccc(OC)cc230)C231CCCCC231CN(Cc232ccc(OC)cc232)C233CCCCC233CN(Cc234ccc(OC)cc234)C235CCCCC235CN(Cc236ccc(OC)cc236)C237CCCCC237CN(Cc238ccc(OC)cc238)C239CCCCC239CN(Cc240ccc(OC)cc240)C241CCCCC241CN(Cc242ccc(OC)cc242)C243CCCCC243CN(Cc244ccc(OC)cc244)C245CCCCC245CN(Cc246ccc(OC)cc246)C247CCCCC247CN(Cc248ccc(OC)cc248)C249CCCCC249CN(Cc250ccc(OC)cc250)C251CCCCC251CN(Cc252ccc(OC)cc252)C253CCCCC253CN(Cc254ccc(OC)cc254)C255CCCCC255CN(Cc256ccc(OC)cc256)C257CCCCC257CN(Cc258ccc(OC)cc258)C259CCCCC259CN(Cc260ccc(OC)cc260)C261CCCCC261CN(Cc262ccc(OC)cc262)C263CCCCC263CN(Cc264ccc(OC)cc264)C265CCCCC265CN(Cc266ccc(OC)cc266)C267CCCCC267CN(Cc268ccc(OC)cc268)C269CCCCC269CN(Cc270ccc(OC)cc270)C271CCCCC271CN(Cc272ccc(OC)cc272)C273CCCCC273CN(Cc274ccc(OC)cc274)C275CCCCC275CN(Cc276ccc(OC)cc276)C277CCCCC277CN(Cc278ccc(OC)cc278)C279CCCCC279CN(Cc280ccc(OC)cc280)C281CCCCC281CN(Cc282ccc(OC)cc282)C283CCCCC283CN(Cc284ccc(OC)cc284)C285CCCCC285CN(Cc286ccc(OC)cc286)C287CCCCC287CN(Cc288ccc(OC)cc288)C289CCCCC289CN(Cc290ccc(OC)cc290)C291CCCCC291CN(Cc292ccc(OC)cc292)C293CCCCC293CN(Cc294ccc(OC)cc294)C295CCCCC295CN(Cc296ccc(OC)cc296)C297CCCCC297CN(Cc298ccc(OC)cc298)C299CCCCC299CN(Cc300ccc(OC)cc300)C301CCCCC301CN(Cc302ccc(OC)cc302)C303CCCCC303CN(Cc304ccc(OC)cc304)C305CCCCC305CN(Cc306ccc(OC)cc306)C307CCCCC307CN(Cc308ccc(OC)cc308)C309CCCCC309CN(Cc310ccc(OC)cc310)C311CCCCC311CN(Cc312ccc(OC)cc312)C313CCCCC313CN(Cc314ccc(OC)cc314)C315CCCCC315CN(Cc316ccc(OC)cc316)C317CCCCC317CN(Cc318ccc(OC)cc318)C319CCCCC319CN(Cc320ccc(OC)cc320)C321CCCCC321CN(Cc322ccc(OC)cc322)C323CCCCC323CN(Cc324ccc(OC)cc324)C325CCCCC325CN(Cc326ccc(OC)cc326)C327CCCCC327CN(Cc328ccc(OC)cc328)C329CCCCC329CN(Cc330ccc(OC)cc330)C331CCCCC331CN(Cc332ccc(OC)cc332)C333CCCCC333CN(Cc334ccc(OC)cc334)C335CCCCC335CN(Cc336ccc(OC)cc336)C337CCCCC337CN(Cc338ccc(OC)cc338)C339CCCCC339CN(Cc340ccc(OC)cc340)C341CCCCC341CN(Cc342ccc(OC)cc342)C343CCCCC343CN(Cc344ccc(OC)cc344)C345CCCCC345CN(Cc346ccc(OC)cc346)C347CCCCC347CN(Cc348ccc(OC)cc348)C349CCCCC349CN(Cc350ccc(OC)cc350)C351CCCCC351CN(Cc352ccc(OC)cc352)C353CCCCC353CN(Cc354ccc(OC)cc354)C355CCCCC355CN(Cc356ccc(OC)cc356)C357CCCCC357CN(Cc358ccc(OC)cc358)C359CCCCC359CN(Cc360ccc(OC)cc360)C361CCCCC361CN(Cc362ccc(OC)cc362)C363CCCCC363CN(Cc364ccc(OC)cc364)C365CCCCC365CN(Cc366ccc(OC)cc366)C367CCCCC367CN(Cc368ccc(OC)cc368)C369CCCCC369CN(Cc370ccc(OC)cc370)C371CCCCC371CN(Cc372ccc(OC)cc372)C373CCCCC373CN(Cc374ccc(OC)cc374)C375CCCCC375CN(Cc376ccc(OC)cc376)C377CCCCC377CN(Cc378ccc(OC)cc378)C379CCCCC379CN(Cc380ccc(OC)cc380)C381CCCCC381CN(Cc382ccc(OC)cc382)C383CCCCC383CN(Cc384ccc(OC)cc384)C385CCCCC385CN(Cc386ccc(OC)cc386)C387CCCCC387CN(Cc388ccc(OC)cc388)C389CCCCC389CN(Cc390ccc(OC)cc390)C391CCCCC391CN(Cc392ccc(OC)cc392)C393CCCCC393CN(Cc394ccc(OC)cc394)C395CCCCC395CN(Cc396ccc(OC)cc396)C397CCCCC397CN(Cc398ccc(OC)cc398)C399CCCCC399CN(Cc400ccc(OC)cc400)C401CCCCC401CN(Cc402ccc(OC)cc402)C403CCCCC403CN(Cc404ccc(OC)cc404)C405CCCCC405CN(Cc406ccc(OC)cc406)C407CCCCC407CN(Cc408ccc(OC)cc408)C409CCCCC409CN(Cc410ccc(OC)cc410)C411CCCCC411CN(Cc412ccc(OC)cc412)C413CCCCC413CN(Cc414ccc(OC)cc414)C415CCCCC415CN(Cc416ccc(OC)cc416)C417CCCCC417CN(Cc418ccc(OC)cc418)C419CCCCC419CN(Cc420ccc(OC)cc420)C421CCCCC421CN(Cc422ccc(OC)cc422)C423CCCCC423CN(Cc424ccc(OC)cc424)C425CCCCC425CN(Cc426ccc(OC)cc426)C427CCCCC427CN(Cc428ccc(OC)cc428)C429CCCCC429CN(Cc430ccc(OC)cc430)C431CCCCC431CN(Cc432ccc(OC)cc432)C433CCCCC433CN(Cc434ccc(OC)cc434)C435CCCCC435CN(Cc436ccc(OC)cc436)C437CCCCC437CN(Cc438ccc(OC)cc438)C439CCCCC439CN(Cc440ccc(OC)cc440)C441CCCCC441CN(Cc442ccc(OC)cc442)C443CCCCC443CN(Cc444ccc(OC)cc444)C445CCCCC445CN(Cc446ccc(OC)cc446)C447CCCCC447CN(Cc448ccc(OC)cc448)C449CCCCC449CN(Cc450ccc(OC)cc450)C451CCCCC451CN(Cc452ccc(OC)cc452)C453CCCCC453CN(Cc454ccc(OC)cc454)C455CCCCC455CN(Cc456ccc(OC)cc456)C457CCCCC457CN(Cc458ccc(OC)cc458)C459CCCCC459CN(Cc460ccc(OC)cc460)C461CCCCC461CN(Cc462ccc(OC)cc462)C463CCCCC463CN(Cc464ccc(OC)cc464)C465CCCCC465CN(Cc466ccc(OC)cc466)C467CCCCC467CN(Cc468ccc(OC)cc468)C469CCCCC469CN(Cc470ccc(OC)cc470)C471CCCCC471CN(Cc472ccc(OC)cc472)C473CCCCC473CN(Cc474ccc(OC)cc474)C475CCCCC475CN(Cc476ccc(OC)cc476)C477CCCCC477CN(Cc478ccc(OC)cc478)C479CCCCC479CN(Cc480ccc(OC)cc480)C481CCCCC481CN(Cc482ccc(OC)cc482)C483CCCCC483CN(Cc484ccc(OC)cc484)C485CCCCC485CN(Cc486ccc(OC)cc486)C487CCCCC487CN(Cc488ccc(OC)cc488)C489CCCCC489CN(Cc490ccc(OC)cc490)C491CCCCC491CN(Cc492ccc(OC)cc492)C493CCCCC493CN(Cc494ccc(OC)cc494)C495CCCCC495CN(Cc496ccc(OC)cc496)C497CCCCC497CN(Cc498ccc(OC)cc498)C499CCCCC499CN(Cc500ccc(OC)cc500)C501CCCCC501CN(Cc502ccc(OC)cc502)C503CCCCC503CN(Cc504ccc(OC)cc504)C505CCCCC505CN(Cc506ccc(OC)cc506)C507CCCCC507CN(Cc508ccc(OC)cc508)C509CCCCC509CN(Cc510ccc(OC)cc510)C511CCCCC511CN(Cc512ccc(OC)cc512)C513CCCCC513CN(Cc514ccc(OC)cc514)C515CCCCC515CN(Cc516ccc(OC)cc516)C517CCCCC517CN(Cc518ccc(OC)cc518)C519CCCCC519CN(Cc520ccc(OC)cc520)C521CCCCC521CN(Cc522ccc(OC)cc522)C523CCCCC523CN(Cc524ccc(OC)cc524)C525CCCCC525CN(Cc526ccc(OC)cc526)C527CCCCC527CN(Cc528ccc(OC)cc528)C529CCCCC529CN(Cc530ccc(OC)cc530)C531CCCCC531CN(Cc532ccc(OC)cc532)C533CCCCC533CN(Cc534ccc(OC)cc534)C535CCCCC535CN(Cc536ccc(OC)cc536)C537CCCCC537CN(Cc538ccc(OC)cc538)C539CCCCC539CN(Cc540ccc(OC)cc540)C541CCCCC541CN(Cc542ccc(OC)cc542)C543CCCCC543CN(Cc544ccc(OC)cc544)C545CCCCC545CN(Cc546ccc(OC)cc546)C547CCCCC547CN(Cc548ccc(OC)cc548)C549CCCCC549CN(Cc550ccc(OC)cc550)C551CCCCC551CN(Cc552ccc(OC)cc552)C553CCCCC553CN(Cc554ccc(OC)cc554)C555CCCCC555CN(Cc556ccc(OC)cc556)C557CCCCC557CN(Cc558ccc(OC)cc558)C559CCCCC559CN(Cc560ccc(OC)cc560)C561CCCCC561CN(Cc562ccc(OC)cc562)C563CCCCC563CN(Cc564ccc(OC)cc564)C565CCCCC565CN(Cc566ccc(OC)cc566)C567CCCCC567CN(Cc568ccc(OC)cc568)C569CCCCC569CN(Cc570ccc(OC)cc570)C571CCCCC571CN(Cc572ccc(OC)cc572)C573CCCCC573CN(Cc574ccc(OC)cc574)C575CCCCC575CN(Cc576ccc(OC)cc576)C577CCCCC577CN(Cc578ccc(OC)cc578)C579CCCCC579CN(Cc580ccc(OC)cc580)C581CCCCC581CN(Cc582ccc(OC)cc582)C583CCCCC583CN(Cc584ccc(OC)cc584)C585CCCCC585CN(Cc586ccc(OC)cc586)C587CCCCC587CN(Cc588ccc(OC)cc588)C589CCCCC589CN(Cc590ccc(OC)cc590)C591CCCCC591CN(Cc592ccc(OC)cc592)C593CCCCC593CN(Cc594ccc(OC)cc594)C595CCCCC595CN(Cc596ccc(OC)cc596)C597CCCCC597CN(Cc598ccc(OC)cc598)C599CCCCC599CN(Cc600ccc(OC)cc600)C601CCCCC601CN(Cc602ccc(OC)cc602)C603CCCCC603CN(Cc604ccc(OC)cc604)C605CCCCC605CN(Cc606ccc(OC)cc606)C607CCCCC607CN(Cc608ccc(OC)cc608)C609CCCCC609CN(Cc610ccc(OC)cc610)C611CCCCC611CN(Cc612ccc(OC)cc612)C613CCCCC613CN(Cc614ccc(OC)cc614)C615CCCCC615CN(Cc616ccc(OC)cc616)C617CCCCC617CN(Cc618ccc(OC)cc618)C619CCCCC619CN(Cc620ccc(OC)cc620)C621CCCCC621CN(Cc622ccc(OC)cc622)C623CCCCC623CN(Cc624ccc(OC)cc624)C625CCCCC625CN(Cc626ccc(OC)cc626)C627CCCCC627CN(Cc628ccc(OC)cc628)C629CCCCC629CN(Cc630ccc(OC)cc630)C631CCCCC631CN(Cc632ccc(OC)cc632)C633CCCCC633CN(Cc634ccc(OC)cc634)C635CCCCC635CN(Cc636ccc(OC)cc636)C637CCCCC637CN(Cc638ccc(OC)cc638)C639CCCCC639CN(Cc640ccc(OC)cc640)C641CCCCC641CN(Cc642ccc(OC)cc642)C643CCCCC643CN(Cc644ccc(OC)cc644)C645CCCCC645CN(Cc646ccc(OC)cc646)C647CCCCC647CN(Cc648ccc(OC)cc648)C649CCCCC649CN(Cc650ccc(OC)cc650)C651CCCCC651CN(Cc652ccc(OC)cc652)C653CCCCC653CN(Cc654ccc(OC)cc654)C655CCCCC655CN(Cc656ccc(OC)cc656)C657CCCCC657CN(Cc658ccc(OC)cc658)C659CCCCC659CN(Cc660ccc(OC)cc660)C661CCCCC661CN(Cc662ccc(OC)cc662)C663CCCCC663CN(Cc664ccc(OC)cc664)C665CCCCC665CN(Cc666ccc(OC)cc666)C667CCCCC667CN(Cc668ccc(OC)cc668)C669CCCCC669CN(Cc670ccc(OC)cc670)C671CCCCC671CN(Cc672ccc(OC)cc672)C673CCCCC673CN(Cc674ccc(OC)cc674)C675CCCCC675CN(Cc676ccc(OC)cc676)C677CCCCC677CN(Cc678ccc(OC)cc678)C679CCCCC679CN(Cc680ccc(OC)cc680)C681CCCCC681CN(Cc682ccc(OC)cc682)C683CCCCC683CN(Cc684ccc(OC)cc684)C685CCCCC685CN(Cc686ccc(OC)cc686)C687CCCCC687CN(Cc688ccc(OC)cc688)C689CCCCC689CN(Cc690ccc(OC)cc690)C691CCCCC691CN(Cc692ccc(OC)cc692)C693CCCCC693CN(Cc694ccc(OC)cc694)C695CCCCC695CN(Cc696ccc(OC)cc696)C697CCCCC697CN(Cc698ccc(OC)cc698)C699CCCCC699CN(Cc700ccc(OC)cc700)C701CCCCC701CN(Cc702ccc(OC)cc702)C703CCCCC703CN(Cc704ccc(OC)cc704)C705CCCCC705CN(Cc706ccc(OC)cc706)C707CCCCC707CN(Cc708ccc(OC)cc708)C709CCCCC709CN(Cc710ccc(OC)cc710)C711CCCCC711CN(Cc712ccc(OC)cc712)C713CCCCC713CN(Cc714ccc(OC)cc714)C715CCCCC715CN(Cc716ccc(OC)cc716)C717CCCCC717CN(Cc718ccc(OC)cc718)C719CCCCC719CN(Cc720ccc(OC)cc720)C721CCCCC721CN(Cc722ccc(OC)cc722)C723CCCCC723CN(Cc724ccc(OC)cc724)C725CCCCC725CN(Cc726ccc(OC)cc726)C727CCCCC727CN(Cc728ccc(OC)cc728)C729CCCCC729CN(Cc730ccc(OC)cc730)C731CCCCC731CN(Cc732ccc(OC)cc732)C733CCCCC733CN(Cc734ccc(OC)cc734)C735CCCCC735CN(Cc736ccc(OC)cc736)C737CCCCC737CN(Cc738ccc(OC)cc738)C739CCCCC739CN(Cc740ccc(OC)cc740)C741CCCCC741CN(Cc742ccc(OC)cc742)C743CCCCC743CN(Cc744ccc(OC)cc744)C745CCCCC745CN(Cc746ccc(OC)cc746)C747CCCCC747CN(Cc748ccc(OC)cc748)C749CCCCC749CN(Cc750ccc(OC)cc750)C751CCCCC751CN(Cc752ccc(OC)cc752)C753CCCCC753CN(Cc754ccc(OC)cc754)C755CCCCC755CN(Cc756ccc(OC)cc756)C757CCCCC757CN(Cc758ccc(OC)cc758)C759CCCCC759CN(Cc760ccc(OC)cc760)C761CCCCC761CN(Cc762ccc(OC)cc762)C763CCCCC763CN(Cc764ccc(OC)cc764)C765CCCCC765CN(Cc766ccc(OC)cc766)C767CCCCC767CN(Cc768ccc(OC)cc768)C769CCCCC769CN(Cc770ccc(OC)cc770)C771CCCCC771CN(Cc772ccc(OC)cc772)C773CCCCC773CN(Cc774ccc(OC)cc774)C775CCCCC775CN(Cc776ccc(OC)cc776)C777CCCCC777CN(Cc778ccc(OC)cc778)C779CCCCC779CN(Cc780ccc(OC)cc780)C781CCCCC781CN(Cc782ccc(OC)cc782)C783CCCCC783CN(Cc784ccc(OC)cc784)C785CCCCC785CN(Cc786ccc(OC)cc786)C787CCCCC787CN(Cc788ccc(OC)cc788)C789CCCCC789CN(Cc790ccc(OC)cc790)C791CCCCC791CN(Cc792ccc(OC)cc792)C793CCCCC793CN(Cc794ccc(OC)cc794)C795CCCCC795CN(Cc796ccc(OC)cc796)C797CCCCC797CN(Cc798ccc(OC)cc798)C799CCCCC799CN(Cc800ccc(OC)cc800)C801CCCCC801CN(Cc802ccc(OC)cc802)C803CCCCC803CN(Cc804ccc(OC)cc804)C805CCCCC805CN(Cc806ccc(OC)cc806)C807CCCCC807CN(Cc808ccc(OC)cc808)C809CCCCC809CN(Cc810ccc(OC)cc810)C811CCCCC811CN(Cc812ccc(OC)cc812)C813CCCCC813CN(Cc814ccc(OC)cc814)C815CCCCC815CN(Cc816ccc(OC)cc816)C817CCCCC817CN(Cc818ccc(OC)cc818)C819CCCCC819CN(Cc820ccc(OC)cc820)C821CCCCC821CN(Cc822ccc(OC)cc822)C823CCCCC823CN(Cc824ccc(OC)cc824)C825CCCCC825CN(Cc826ccc(OC)cc826)C827CCCCC827CN(Cc828ccc(OC)cc828)C829CCCCC829CN(Cc830ccc(OC)cc830)C831CCCCC831CN(Cc832ccc(OC)cc832)C833CCCCC833CN(Cc834ccc(OC)cc834)C835CCCCC835CN(Cc836ccc(OC)cc836)C837CCCCC837CN(Cc838ccc(OC)cc838)C839CCCCC839CN(Cc840ccc(OC)cc840)C841CCCCC841CN(Cc842ccc(OC)cc842)C843CCCCC843CN(Cc844ccc(OC)cc844)C845CCCCC845CN(Cc846ccc(OC)cc846)C847CCCCC847CN(Cc848ccc(OC)cc848)C849CCCCC849CN(Cc850ccc(OC)cc850)C851CCCCC851CN(Cc852ccc(OC)cc852)C853CCCCC853CN(Cc854ccc(OC)cc854)C855CCCCC855CN(Cc856ccc(OC)cc856)C857CCCCC857CN(Cc858ccc(OC)cc858)C859CCCCC859CN(Cc860ccc(OC)cc860)C861CCCCC861CN(Cc862ccc(OC)cc862)C863CCCCC863CN(Cc864ccc(OC)cc864)C865CCCCC865CN(Cc866ccc(OC)cc866)C867CCCCC867CN(Cc868ccc(OC)cc868)C869CCCCC869CN(Cc870ccc(OC)cc870)C871CCCCC871CN(Cc872ccc(OC)cc872)C873CCCCC873CN(Cc874ccc(OC)cc874)C875CCCCC875CN(Cc876ccc(OC)cc876)C877CCCCC877CN(Cc878ccc(OC)cc878)C879CCCCC879CN(Cc880ccc(OC)cc880)C881CCCCC881CN(Cc882ccc(OC)cc882)C883CCCCC883CN(Cc884ccc(OC)cc884)C885CCCCC885CN(Cc886ccc(OC)cc886)C887CCCCC887CN(Cc888ccc(OC)cc888)C889CCCCC889CN(Cc890ccc(OC)cc890)C891CCCCC891CN(Cc892ccc(OC)cc892)C893CCCCC893CN(Cc894ccc(OC)cc894)C895CCCCC895CN(Cc896ccc(OC)cc896)C897CCCCC897CN(Cc898ccc(OC)cc898)C899CCCCC899CN(Cc900ccc(OC)cc900)C901CCCCC901CN(Cc902ccc(OC)cc902)C903CCCCC903CN(Cc904ccc(OC)cc904)C905CCCCC905CN(Cc906ccc(OC)cc906)C907CCCCC907CN(Cc908ccc(OC)cc908)C909CCCCC909CN(Cc910ccc(OC)cc910)C911CCCCC911CN(Cc912ccc(OC)cc912)C913CCCCC913CN(Cc914ccc(OC)cc914)C915CCCCC915CN(Cc916ccc(OC)cc916)C917CCCCC917CN(Cc918ccc(OC)cc918)C919CCCCC919CN(Cc920ccc(OC)cc920)C921CCCCC921CN(Cc922ccc(OC)cc922)C923CCCCC923CN(Cc924ccc(OC)cc924)C925CCCCC925CN(Cc926ccc(OC)cc926)C927CCCCC927CN(Cc928ccc(OC)cc928)C929CCCCC929CN(Cc930ccc(OC)cc930)C931CCCCC931CN(Cc932ccc(OC)cc932)C933CCCCC933CN(Cc934ccc(OC)cc934)C935CCCCC935CN(Cc936ccc(OC)cc936)C937CCCCC937CN(Cc938ccc(OC)cc938)C939CCCCC939CN(Cc940ccc(OC)cc940)C941CCCCC941CN(Cc942ccc(OC)cc942)C943CCCCC943CN(Cc944ccc(OC)cc944)C945CCCCC945CN(Cc946ccc(OC)cc946)C947CCCCC947CN(Cc948ccc(OC)cc948)C949CCCCC949CN(Cc950ccc(OC)cc950)C951CCCCC951CN(Cc952ccc(OC)cc952)C953CCCCC953CN(Cc954ccc(OC)cc954)C955CCCCC955CN(Cc956ccc(OC)cc956)C957CCCCC957CN(Cc958ccc(OC)cc958)C959CCCCC959CN(Cc960ccc(OC)cc960)C961CCCCC961CN(Cc962ccc(OC)cc962)C963CCCCC963CN(Cc964ccc(OC)cc964)C965CCCCC965CN(Cc966ccc(OC)cc966)C967CCCCC967CN(Cc968ccc(OC)cc968)C969CCCCC969CN(Cc970ccc(OC)cc970)C971CCCCC971CN(Cc972ccc(OC)cc972)C973CCCCC973CN(Cc974ccc(OC)cc974)C975CCCCC975CN(Cc976ccc(OC)cc976)C977CCCCC977CN(Cc978ccc(OC)cc978)C979CCCCC979CN(Cc980ccc(OC)cc980)C981CCCCC981CN(Cc982ccc(OC)cc982)C983CCCCC983CN(Cc984ccc(OC)cc984)C985CCCCC985CN(Cc986ccc(OC)cc986)C987CCCCC987CN(Cc988ccc(OC)cc988)C989CCCCC989CN(Cc990ccc(OC)cc990)C991CCCCC991CN(Cc992ccc(OC)cc992)C993CCCCC993CN(Cc994ccc(OC)cc994)C995CCCCC995CN(Cc996ccc(OC)cc996)C997CCCCC997CN(Cc998ccc(OC)cc998)C999CCCCC999CN(Cc1000ccc(OC)cc1000)C1001CCCCC1001CN(Cc1002ccc(OC)cc1002)C1003CCCCC1003CN(Cc1004ccc(OC)cc1004)C1005CCCCC1005CN(Cc1006ccc(OC)cc1006)C1007CCCCC1007CN(Cc1008ccc(OC)cc1008)C1009CCCCC1009CN(Cc1010ccc(OC)cc1010)C1011CCCCC1011CN(Cc1012ccc(OC)cc1012)C1013CCCCC1013CN(Cc1014ccc(OC)cc1014)C1015CCCCC1015CN(Cc1016ccc(OC)cc1016)C1017CCCCC1017CN(Cc1018ccc(OC)cc1018)C1019CCCCC1019</chem>		

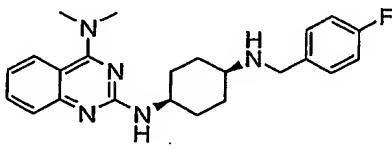
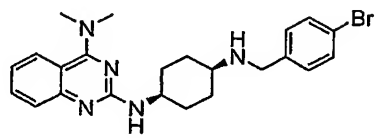
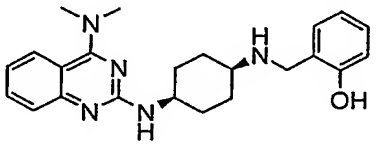
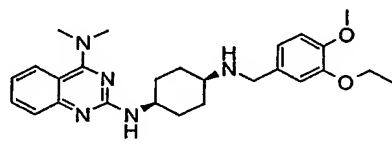
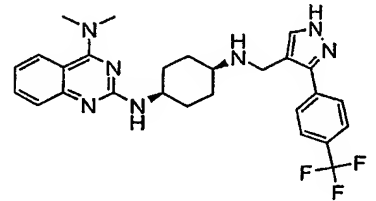
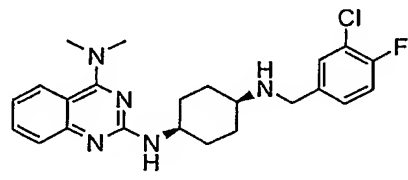
Example No.	Structure	ESI-MS	Retention Time (min)
3221	 $2\text{CF}_3\text{CO}_2\text{H}$	478.4 (M + H)	3.17
3222	 $2\text{CF}_3\text{CO}_2\text{H}$	480.0 (M + H)	3.08
3223	 $2\text{CF}_3\text{CO}_2\text{H}$	590.2 (M + H)	4.20
3224	 $2\text{CF}_3\text{CO}_2\text{H}$	576.4 (M + H)	3.95
3225	 $2\text{CF}_3\text{CO}_2\text{H}$	512.4 (M + H)	3.86
3226	 $\text{CF}_3\text{CO}_2\text{H}$	472.4 (M + H)	3.07

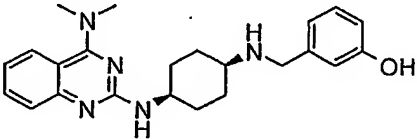
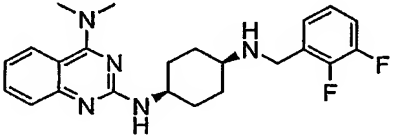
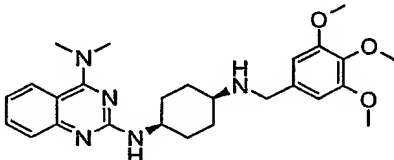
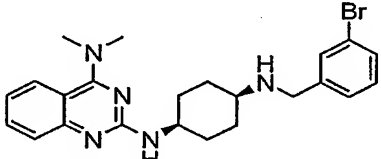
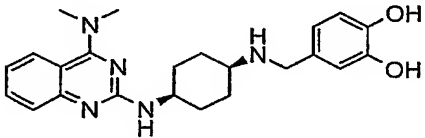
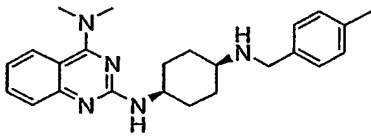
Example No.	Structure	ESI-MS	Retention Time (min)
3227	 $\text{CF}_3\text{CO}_2\text{H}$	540.6 (M + H)	3.75
3228	 $\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	3.07
3229	 $2\text{CF}_3\text{CO}_2\text{H}$	478.4 (M + H)	3.40
3230	 $2\text{CF}_3\text{CO}_2\text{H}$	552.6 (M + H)	3.50
3231	 $2\text{CF}_3\text{CO}_2\text{H}$	590.2 (M + H)	3.60
3232	 $2\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	3.25

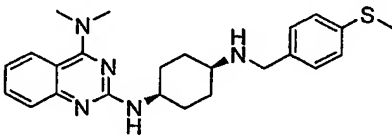
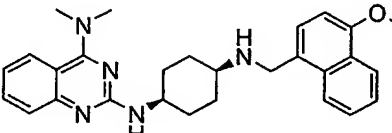
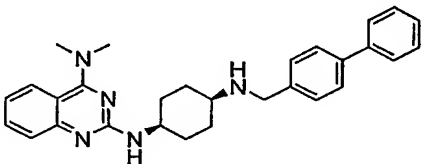
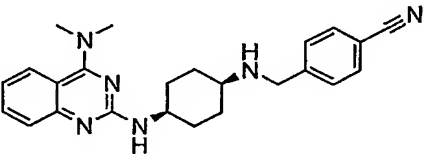
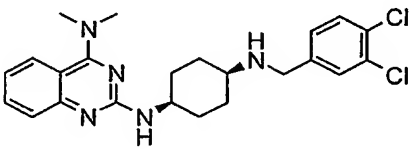
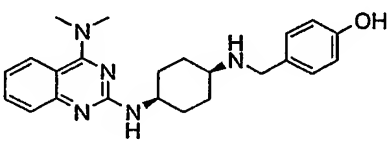
Example No.	Structure	ESI-MS	Retention Time (min)
3233	 $2\text{CF}_3\text{CO}_2\text{H}$	382.2 (M + H)	2.67
3234	 $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	3.05
3235	 $2\text{CF}_3\text{CO}_2\text{H}$	394.4 (M + H)	2.75
3236	 $2\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.82
3237	 $2\text{CF}_3\text{CO}_2\text{H}$	426.4 (M + H)	3.17
3238	 $2\text{CF}_3\text{CO}_2\text{H}$	468.4 (M + H)	3.44

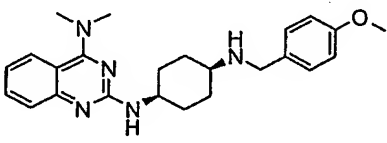
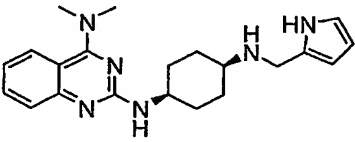
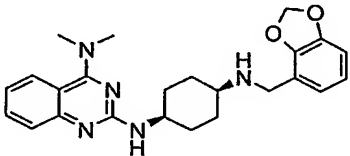
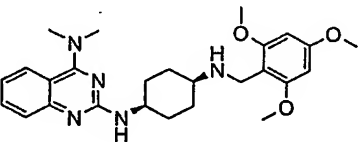
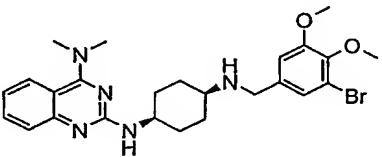
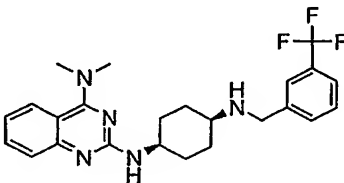
Example No.	Structure	ESI-MS	Retention Time (min)
3239	 <chem>CN(C)c1nc2c(ncn2C1)C3=CC=CC=C3N[C@H]4CCCC[C@H]4NCc5cc(OC)c(O)c(OC)c5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	452.2 (M + H)	2.69
3240	 <chem>CN(C)c1nc2c(ncn2C1)C3=CC=CC=C3N[C@H]4CCCC[C@H]4NCc5cc(OC)c(O)c(O)c5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	2.80
3241	 <chem>CN(C)c1nc2c(ncn2C1)C3=CC=CC=C3N[C@H]4CCCC[C@H]4NCc5cc(O)c(Cl)ccc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	2.79
3242	 <chem>CN(C)c1nc2c(ncn2C1)C3=CC=CC=C3N[C@H]4CCCC[C@H]4NCc5ccc(Oc6ccc(Cl)cc6)cc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	536.4 (M + H)	3.75
3243	 <chem>CN(C)c1nc2c(ncn2C1)C3=CC=CC=C3N[C@H]4CCCC[C@H]4NCc5cnc6ccccc6n5</chem> $3\text{CF}_3\text{CO}_2\text{H}$	427.2 (M + H)	2.95
3244	 <chem>CN(C)c1nc2c(ncn2C1)C3=CC=CC=C3N[C@H]4CCCC[C@H]4NCc5ccc(C(C)(C)C)cc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	432.4 (M + H)	3.41

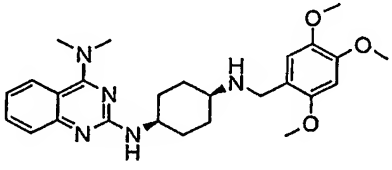
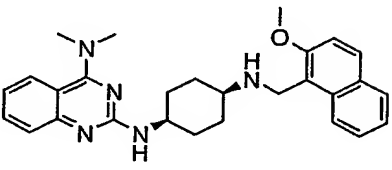
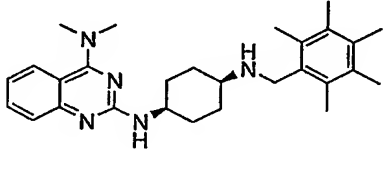
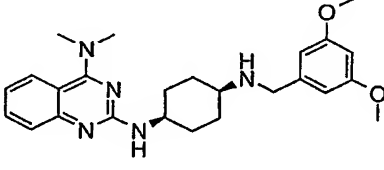
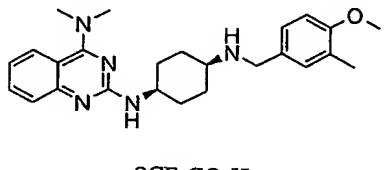

Example No.	Structure	ESI-MS	Retention Time (min)
3245	 <chem>CC1=NC2=CC=CC=C2N(C)N1C3=CC=CC=C3N3</chem> <chem>COc1ccc(cc1)CN[C@H]2CCCC[C@H]2N3C=NC4=CC=CC=C4N(C)N3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	434.2 (M + H)	2.84
3246	 <chem>Clc1ccc(cc1)CN[C@H]2CCCC[C@H]2N3C=NC4=CC=CC=C4N(C)N3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	410.2 (M + H)	3.02
3247	 <chem>c1ccc2nc(ccc2c1)CCN[C@H]3CCCC[C@H]3N4C=NC5=CC=CC=C5N(C)N4</chem> $3\text{CF}_3\text{CO}_2\text{H}$	427.4 (M + H)	2.61
3248	 <chem>COC1=CC=C(C=C1)C2=CC=CC=C2O2</chem> <chem>CC1=NC2=CC=CC=C2N(C)N1C3=CC=CC=C3N3</chem> <chem>COC1=CC=C(C=C1)C2=CC=CC=C2O2CN[C@H]4CCCC[C@H]4N5C=NC6=CC=CC=C6N(C)N5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	2.91
3249	 <chem>FC(F)(F)Oc1ccc(cc1)CN[C@H]2CCCC[C@H]2N3C=NC4=CC=CC=C4N(C)N3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	460.4 (M + H)	3.19
3250	 <chem>c1ccc(cc1)Oc2ccc(cc2)CN[C@H]3CCCC[C@H]3N4C=NC5=CC=CC=C5N(C)N4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	468.4 (M + H)	2.79

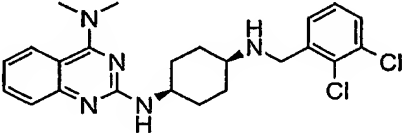
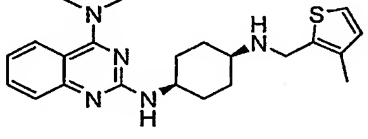
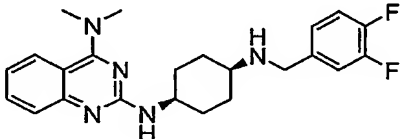
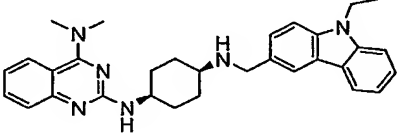
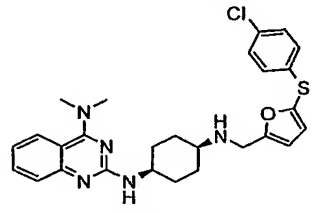
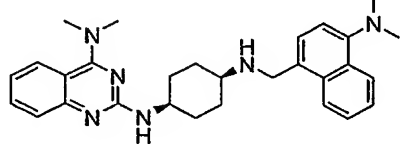
Example No.	Structure	ESI-MS	Retention Time (min)
3251	 $2\text{CF}_3\text{CO}_2\text{H}$	394.4 (M + H)	2.83
3252	 $2\text{CF}_3\text{CO}_2\text{H}$	454.2 (M + H)	3.08
3253	 $2\text{CF}_3\text{CO}_2\text{H}$	392.4 (M + H)	2.73
3254	 $2\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	2.92
3255	 $3\text{CF}_3\text{CO}_2\text{H}$	510.4 (M + H)	3.17
3256	 $2\text{CF}_3\text{CO}_2\text{H}$	428.2 (M + H)	3.08

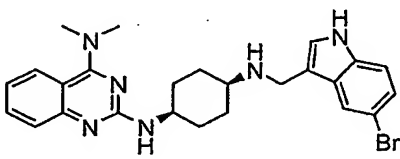
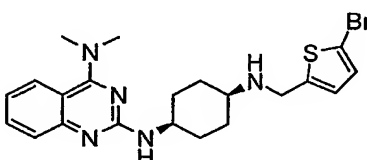
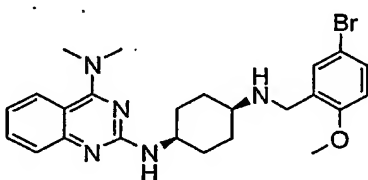
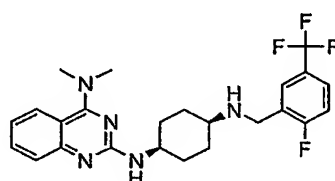
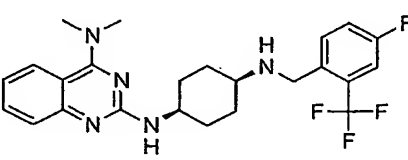
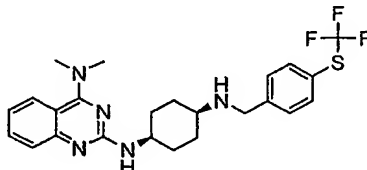
Example No.	Structure	ESI-MS	Retention Time (min)
3257	 $2\text{CF}_3\text{CO}_2\text{H}$	392.4 (M + H)	2.63
3258	 $2\text{CF}_3\text{CO}_2\text{H}$	412.2 (M + H)	2.83
3259	 $2\text{CF}_3\text{CO}_2\text{H}$	466.4 (M + H)	2.89
3260	 $2\text{CF}_3\text{CO}_2\text{H}$	454.0 (M + H)	3.05
3261	 $2\text{CF}_3\text{CO}_2\text{H}$	408.2 (M + H)	2.53
3262	 $2\text{CF}_3\text{CO}_2\text{H}$	390.4 (M + H)	2.92

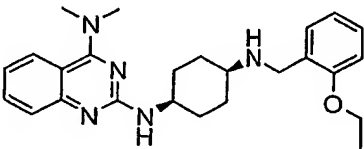
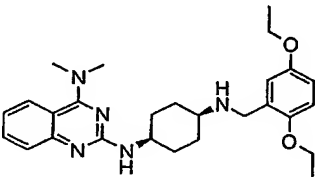
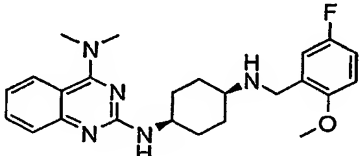
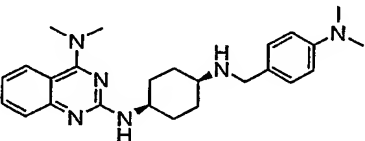
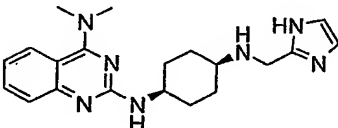
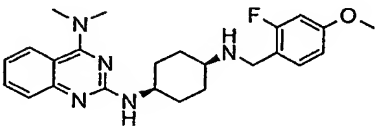
Example No.	Structure	ESI-MS	Retention Time (min)
3263	 <chem>CN(C)c1nc2c(ncn2C1NCCc3ccc(SC)cc3)c3ccccc3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	422.2 (M + H)	3.05
3264	 <chem>CN(C)c1nc2c(ncn2C1NCCc3ccc(OC)cc3)c3ccccc3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	456.4 (M + H)	3.25
3265	 <chem>CN(C)c1nc2c(ncn2C1NCCc3ccc(cc3)-c4ccccc4)c3ccccc3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	452.2 (M + H)	3.37
3266	 <chem>CN(C)c1nc2c(ncn2C1NCCc3ccc(C#N)cc3)c3ccccc3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	401.2 (M + H)	2.76
3267	 <chem>CN(C)c1nc2c(ncn2C1NCCc3cc(Cl)c(Cl)cc3)c3ccccc3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	444.4 (M + H)	3.17
3268	 <chem>CN(C)c1nc2c(ncn2C1NCCc3ccc(O)cc3)c3ccccc3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	392.4 (M + H)	2.61

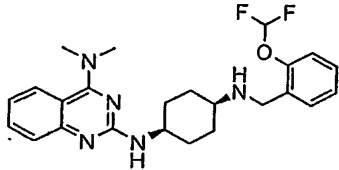
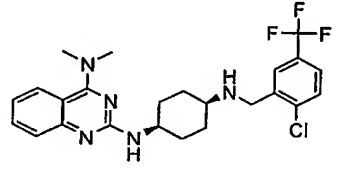
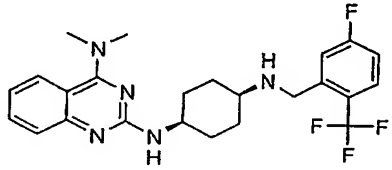
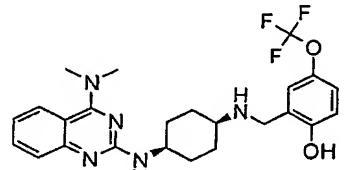
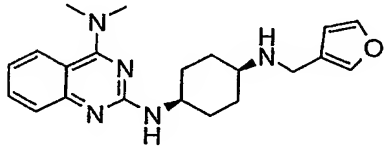
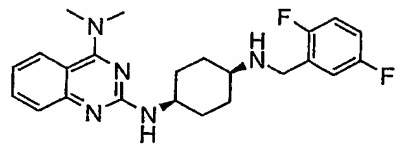
Example No.	Structure	ESI-MS	Retention Time (min)
3269	 $2\text{CF}_3\text{CO}_2\text{H}$	406.4 (M + H)	2.86
3270	 $3\text{CF}_3\text{CO}_2\text{H}$	365.4 (M + H)	2.61
3271	 $2\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.83
3272	 $2\text{CF}_3\text{CO}_2\text{H}$	466.4 (M + H)	3.10
3273	 $2\text{CF}_3\text{CO}_2\text{H}$	514.4 (M + H)	3.13
3274	 $2\text{CF}_3\text{CO}_2\text{H}$	444.4 (M + H)	3.17

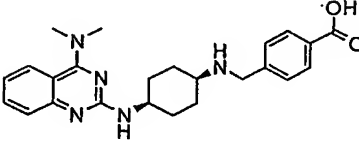
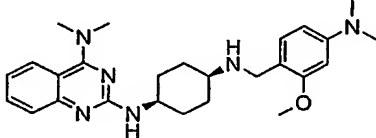
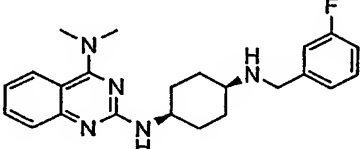
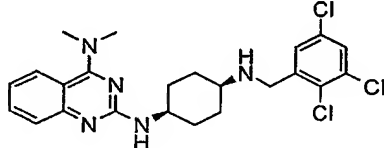
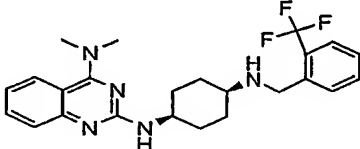
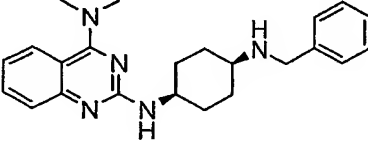
Example No.	Structure	ESI-MS	Retention Time (min)
3275	 2CF ₃ CO ₂ H	466.4 (M + H)	2.86
3276	 2CF ₃ CO ₂ H	456.2 (M + H)	3.22
3277	 2CF ₃ CO ₂ H	446.6 (M + H)	3.45
3278	 2CF ₃ CO ₂ H	436.4 (M + H)	2.95
3279	 2CF ₃ CO ₂ H	420.2 (M + H)	3.03
3280	 2CF ₃ CO ₂ H	382.4 (M + H)	2.72

Example No.	Structure	ESI-MS	Retention Time (min)
3281	 $2\text{CF}_3\text{CO}_2\text{H}$	444.4 (M + H)	3.07
3282	 $2\text{CF}_3\text{CO}_2\text{H}$	396.2 (M + H)	2.79
3283	 $2\text{CF}_3\text{CO}_2\text{H}$	412.4 (M + H)	2.95
3284	 $32\text{CF}_3\text{CO}_2\text{H}$	493.4 (M + H)	3.57
3285	 $2\text{CF}_3\text{CO}_2\text{H}$	508.2 (M + H)	3.52
3286	 $2\text{CF}_3\text{CO}_2\text{H}$	469.6 (M + H)	2.76

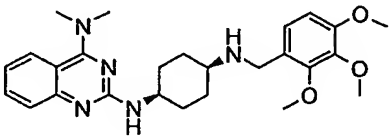
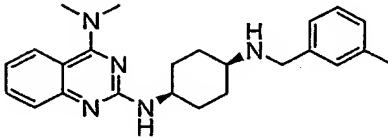
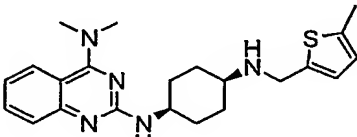
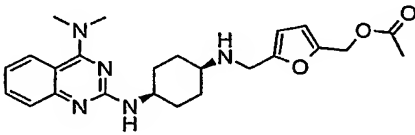
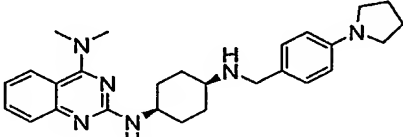
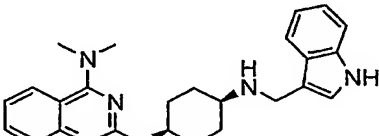
Example No.	Structure	ESI-MS	Retention Time (min)
3287	 $3\text{CF}_3\text{CO}_2\text{H}$	493.2 (M + H)	3.17
3288	 $2\text{CF}_3\text{CO}_2\text{H}$	460.2 (M + H)	2.95
3289	 $2\text{CF}_3\text{CO}_2\text{H}$	484.2 (M + H)	3.14
3290	 $2\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	3.11
3291	 $2\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	3.11
3292	 $2\text{CF}_3\text{CO}_2\text{H}$	476.4 (M + H)	3.39

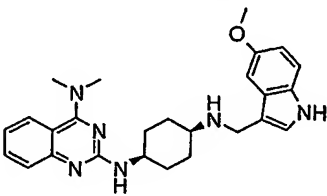
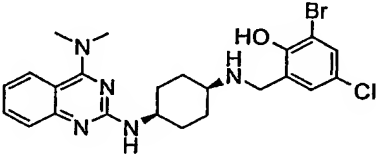
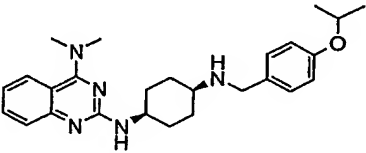
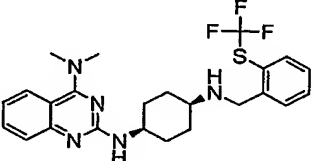
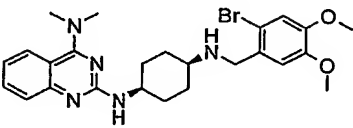
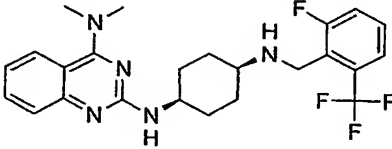
Example No.	Structure	ESI-MS	Retention Time (min)
3293	 $2\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	3.05
3294	 $2\text{CF}_3\text{CO}_2\text{H}$	464.2 (M + H)	3.21
3295	 $2\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	2.94
3296	 $3\text{CF}_3\text{CO}_2\text{H}$	419.4 (M + H)	2.51
3297	 $3\text{CF}_3\text{CO}_2\text{H}$	366.4 (M + H)	2.26
3298	 $2\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	2.93

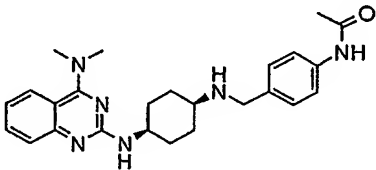
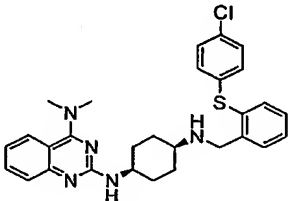
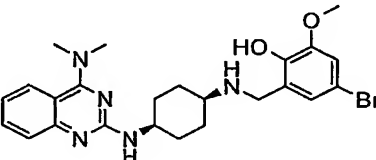
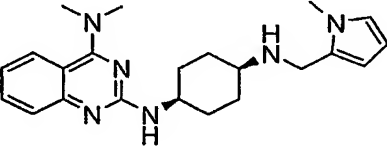
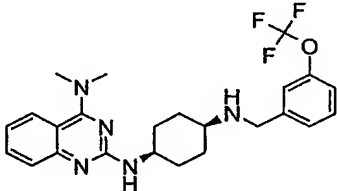
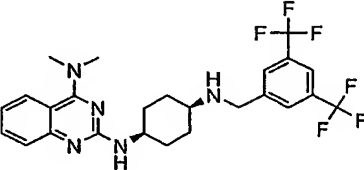
Example No.	Structure	ESI-MS	Retention Time (min)
3299	 <chem>CN(C)c1nc2c(ncn2C1)C3CCCCC3CNc4cc(OC(F)(F)F)ccc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	442.4 (M + H)	2.97
3300	 <chem>CN(C)c1nc2c(ncn2C1)C3CCCCC3CNc4cc(C(F)(F)F)c(Cl)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	478.2 (M + H)	3.19
3301	 <chem>CN(C)c1nc2c(ncn2C1)C3CCCCC3CNc4cc(C(F)(F)F)c(F)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	3.05
3302	 <chem>CN(C)c1nc2c(ncn2C1)C3CCCCC3CNc4cc(OC(F)(F)F)c(O)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	476.4 (M + H)	3.20
3303	 <chem>CN(C)c1nc2c(ncn2C1)C3CCCCC3CNc4ccoc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	366.4 (M + H)	2.64
3304	 <chem>CN(C)c1nc2c(ncn2C1)C3CCCCC3CNc4cc(F)ccc4F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	412.4 (M + H)	2.85

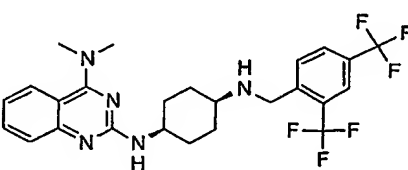
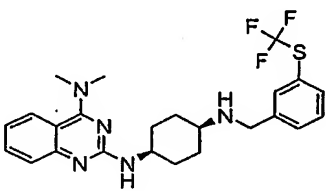
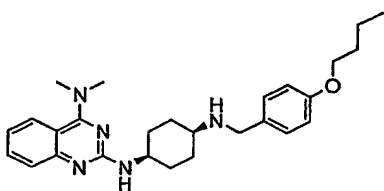
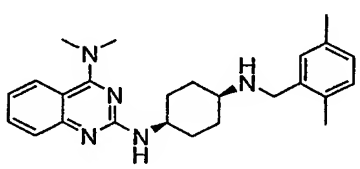
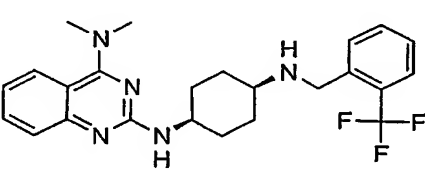
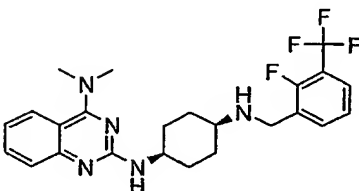
Example No.	Structure	ESI-MS	Retention Time (min)
3305	 2CF ₃ CO ₂ H	420.4 (M + H)	2.67
3306	 3CF ₃ CO ₂ H	449.4 (M + H)	2.74
3307	 2CF ₃ CO ₂ H	394.4 (M + H)	2.86
3308	 2CF ₃ CO ₂ H	478.2 (M + H)	3.38
3309	 2CF ₃ CO ₂ H	444.4 (M + H)	3.09
3310	 2CF ₃ CO ₂ H	376.4 (M + H)	2.82

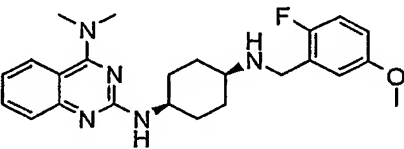
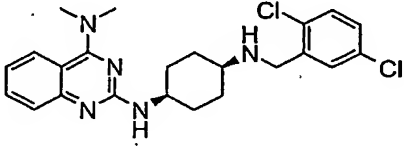
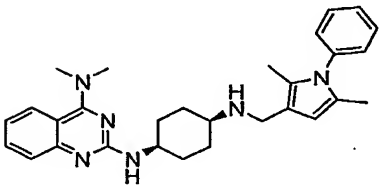
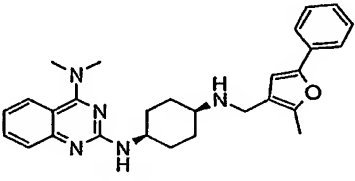
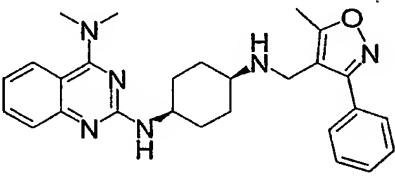
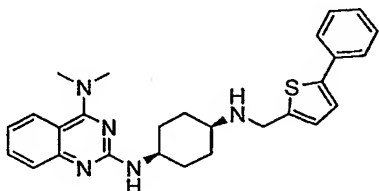
Example No.	Structure	ESI-MS	Retention Time (min)
3311	 <chem>CN(C)c1nc2c(ncn2C1NCC3=CC=CC=C3OC)C4=CC=CC=C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	406.4 (M + H)	2.87
3312	 <chem>CN(C)c1nc2c(ncn2C1NCC3=CC(OC)=CC(OC)=C3)C4=CC=CC=C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	2.91
3313	 <chem>CN(C)c1nc2c(ncn2C1NCC3=CC4=CC=CC=C4C=C3)C4=CC=CC=C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	3.13
3314	 <chem>CN(C)c1nc2c(ncn2C1NCC3=CC(OC)=CC(OC)=C3)C4=CC=CC=C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	2.99
3315	 <chem>CN(C)c1nc2c(ncn2C1NCC3=CC=CC=C3Br)C4=CC=CC=C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	454.0 (M + H)	2.97
3316	 <chem>CN(C)c1nc2c(ncn2C1NCC3=CC(F)=CC(F)=C3)C4=CC=CC=C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	412.4 (M + H)	2.92

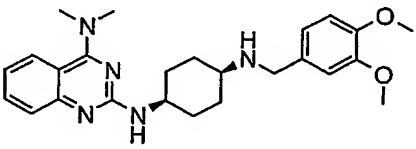
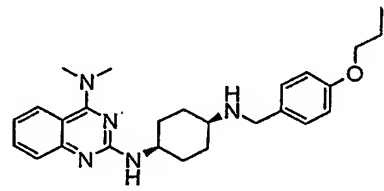
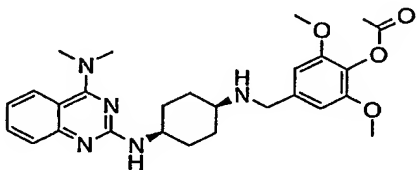
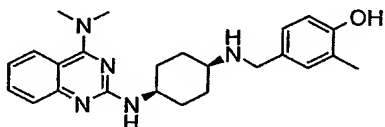
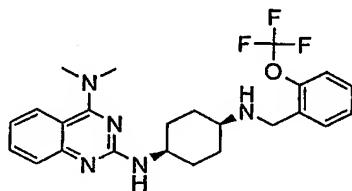
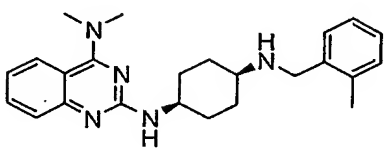
Example No.	Structure	ESI-MS	Retention Time (min)
3317	 $2\text{CF}_3\text{CO}_2\text{H}$	466.4 (M + H)	2.95
3318	 $2\text{CF}_3\text{CO}_2\text{H}$	390.4 (M + H)	2.95
3319	 $2\text{CF}_3\text{CO}_2\text{H}$	396.2 (M + H)	2.89
3320	 $2\text{CF}_3\text{CO}_2\text{H}$	438.2 (M + H)	2.76
3321	 $3\text{CF}_3\text{CO}_2\text{H}$	445.4 (M + H)	3.16
3322	 $3\text{CF}_3\text{CO}_2\text{H}$	415.4 (M + H)	2.96

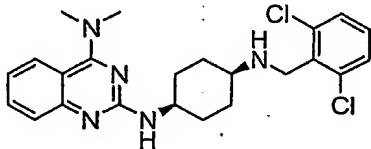
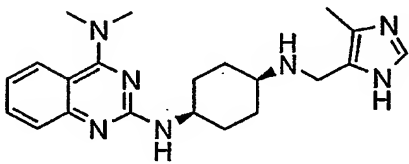
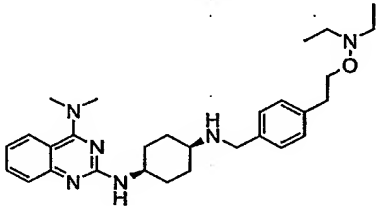
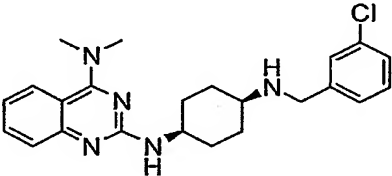
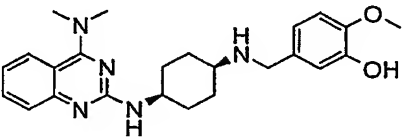
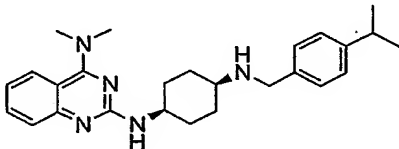
Example No.	Structure	ESI-MS	Retention Time (min)
3323	 $3\text{CF}_3\text{CO}_2\text{H}$	445.4 (M + H)	2.96
3324	 $2\text{CF}_3\text{CO}_2\text{H}$	504.2 (M + H)	3.11
3325	 $2\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	3.17
3326	 $2\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	3.27
3327	 $2\text{CF}_3\text{CO}_2\text{H}$	514.4 (M + H)	3.07
3328	 $2\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	2.99

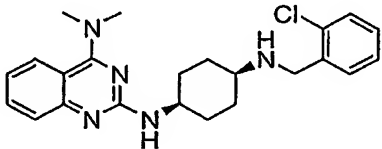
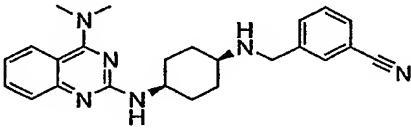
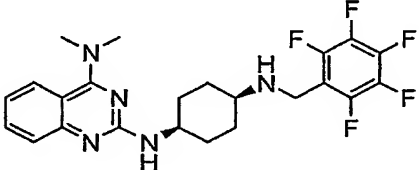
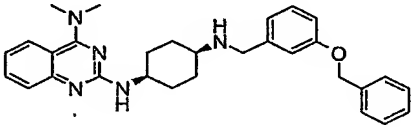
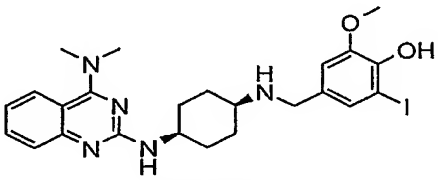
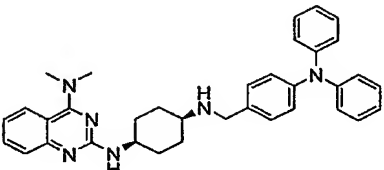
Example No.	Structure	ESI-MS	Retention Time (min)
3329	 $2\text{CF}_3\text{CO}_2\text{H}$	433.2 (M + H)	2.63
3330	 $2\text{CF}_3\text{CO}_2\text{H}$	518.4 (M + H)	3.63
3331	 $2\text{CF}_3\text{CO}_2\text{H}$	500.4 (M + H)	3.09
3332	 $3\text{CF}_3\text{CO}_2\text{H}$	379.4 (M + H)	2.77
3333	 $2\text{CF}_3\text{CO}_2\text{H}$	460.2 (M + H)	3.31
3334	 $2\text{CF}_3\text{CO}_2\text{H}$	512.4 (M + H)	3.51

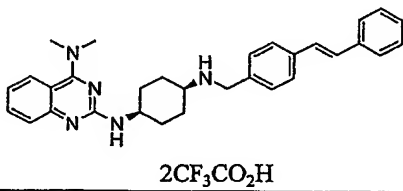
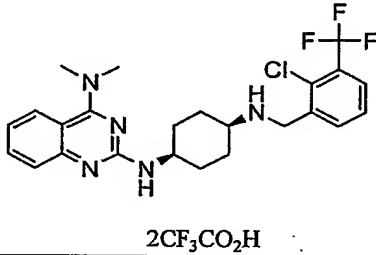
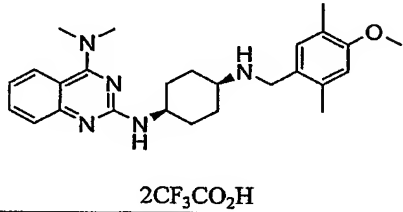
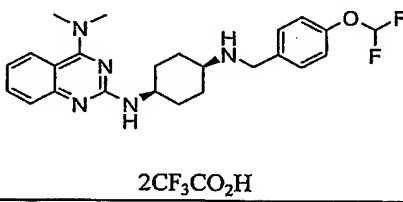
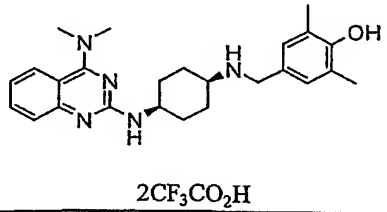
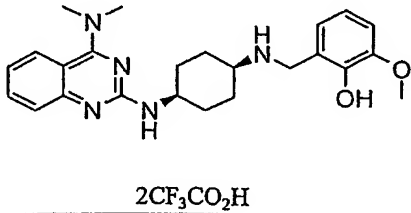
Example No.	Structure	ESI-MS	Retention Time (min)
3335	 2CF ₃ CO ₂ H	512.6 (M + H)	3.51
3336	 2CF ₃ CO ₂ H	476.2 (M + H)	3.39
3337	 2CF ₃ CO ₂ H	448.4 (M + H)	3.42
3338	 2CF ₃ CO ₂ H	404.4 (M + H)	3.17
3339	 2CF ₃ CO ₂ H	444.4 (M + H)	3.13
3340	 2CF ₃ CO ₂ H	462.2 (M + H)	3.21

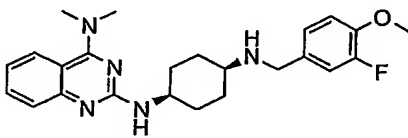
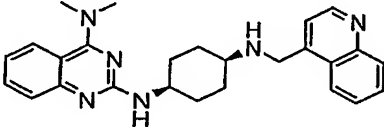
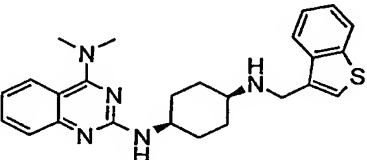
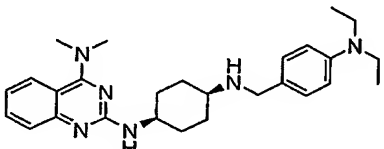
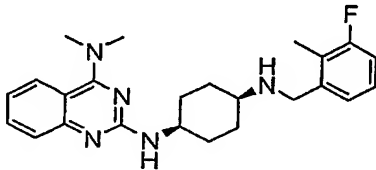
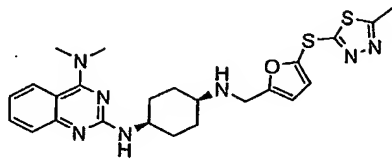
Example No.	Structure	ESI-MS	Retention Time (min)
3341	 2CF ₃ CO ₂ H	424.2 (M + H)	2.97
3342	 2CF ₃ CO ₂ H	444.6 (M + H)	3.16
3343	 3CF ₃ CO ₂ H	469.4 (M + H)	3.47
3344	 2CF ₃ CO ₂ H	456.4 (M + H)	3.47
3345	 2CF ₃ CO ₂ H	457.4 (M + H)	3.09
3346	 2CF ₃ CO ₂ H	458.2 (M + H)	3.37

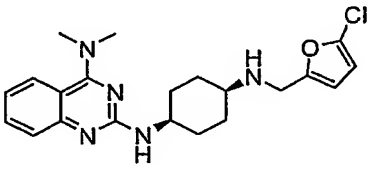
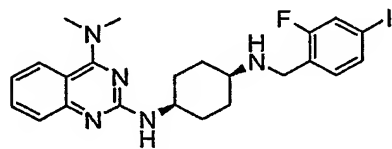
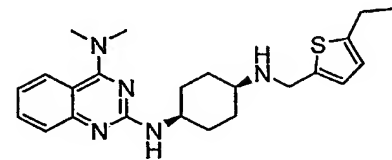
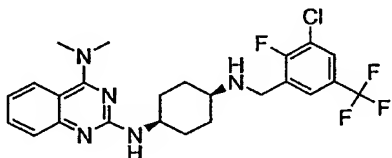
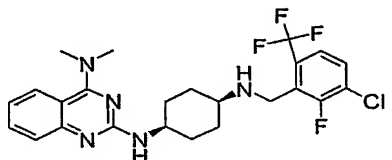
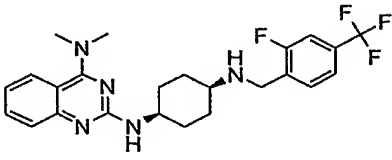
Example No.	Structure	ESI-MS	Retention Time (min)
3347	 $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	2.83
3348	 $2\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	3.30
3349	 $2\text{CF}_3\text{CO}_2\text{H}$	494.4 (M + H)	2.98
3350	 $2\text{CF}_3\text{CO}_2\text{H}$	406.4 (M + H)	2.80
3351	 $2\text{CF}_3\text{CO}_2\text{H}$	460.4 (M + H)	3.20
3352	 $2\text{CF}_3\text{CO}_2\text{H}$	390.4 (M + H)	2.97

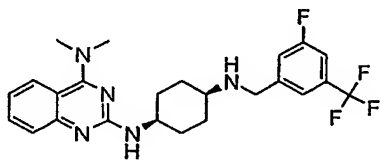
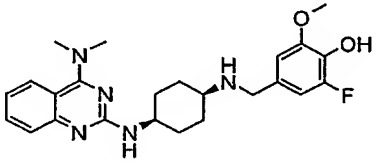
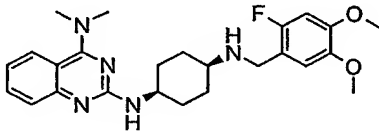
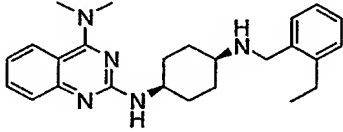
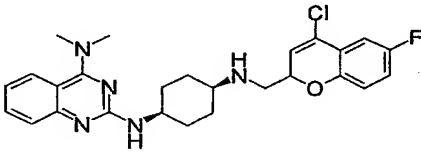
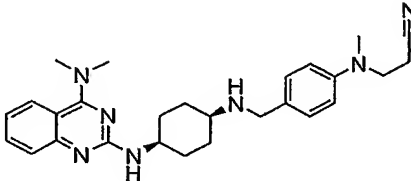
Example No.	Structure	ESI-MS	Retention Time (min)
3353	 $2\text{CF}_3\text{CO}_2\text{H}$	444.2 (M + H)	3.01
3354	 $3\text{CF}_3\text{CO}_2\text{H}$	380.2 (M + H)	2.27
3355	 $2\text{CF}_3\text{CO}_2\text{H}$	491.4 (M + H)	2.55
3356	 $2\text{CF}_3\text{CO}_2\text{H}$	410.4 (M + H)	3.05
3357	 $2\text{CF}_3\text{CO}_2\text{H}$	422.2 (M + H)	2.69
3358	 $2\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	3.36

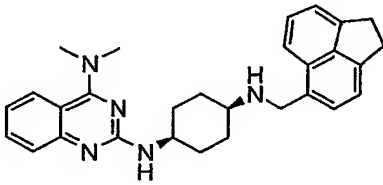
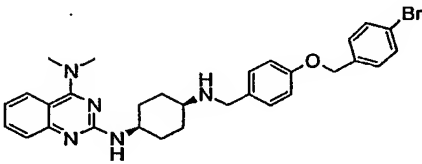
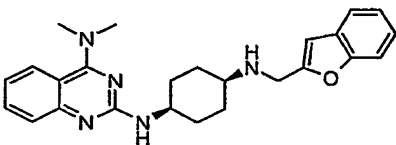
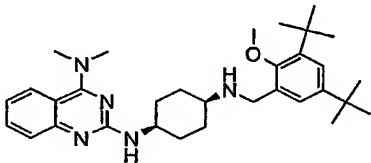
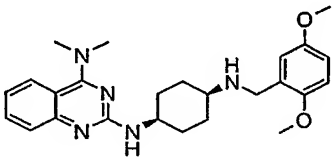
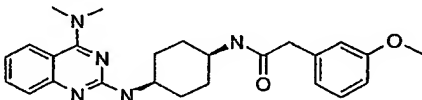
Example No.	Structure	ESI-MS	Retention Time (min)
3359	 <chem>CN(C)c1nc2c(ncn2C1NCC3CCCCC3NCC4=CC=CC=C4Cl)C5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	410.4 (M + H)	2.97
3360	 <chem>CN(C)c1nc2c(ncn2C1NCC3CCCCC3NCC4=CC=C(C#N)C=C4)C5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	401.2 (M + H)	2.81
3361	 <chem>CN(C)c1nc2c(ncn2C1NCC3CCCCC3NCC4=C(F)C(F)=C(F)C(F)=C4)C5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	466.2 (M + H)	3.01
3362	 <chem>CN(C)c1nc2c(ncn2C1NCC3CCCCC3NCC4=CC=C(OC5=CC=CC=C5)C=C4)C6=CC=CC=C6</chem> $2\text{CF}_3\text{CO}_2\text{H}$	482.4 (M + H)	3.43
3363	 <chem>CN(C)c1nc2c(ncn2C1NCC3CCCCC3NCC4=CC(=C(C=C4)O)I)C5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	548.4 (M + H)	3.03
3364	 <chem>CN(C)c1nc2c(ncn2C1NCC3CCCCC3NCC4=CC=C(N(C5=CC=CC=C5)C6=CC=CC=C6)C=C4)C7=CC=CC=C7</chem> $3\text{CF}_3\text{CO}_2\text{H}$	543.6 (M + H)	3.95

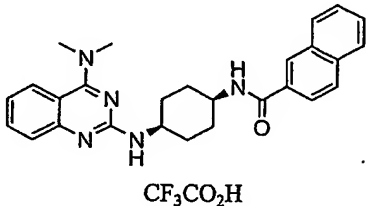
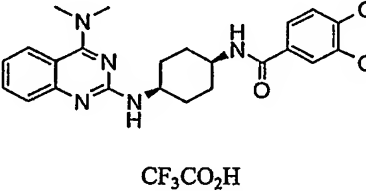
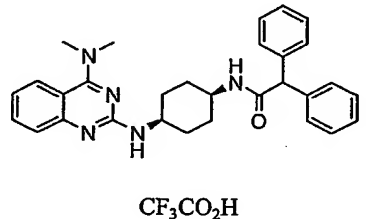
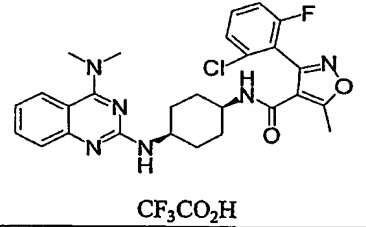
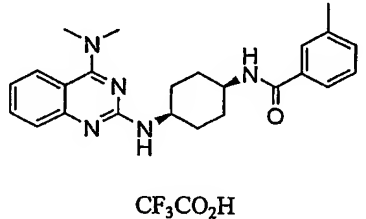
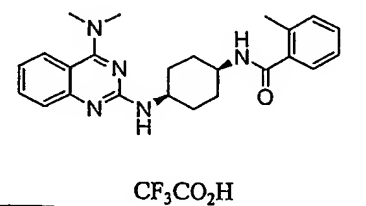
Example No.	Structure	ESI-MS	Retention Time (min)
3365	 2CF ₃ CO ₂ H	478.4 (M + H)	3.64
3366	 2CF ₃ CO ₂ H	478.4 (M + H)	3.29
3367	 2CF ₃ CO ₂ H	434.4 (M + H)	3.20
3368	 2CF ₃ CO ₂ H	442.4 (M + H)	3.09
3369	 2CF ₃ CO ₂ H	420.4 (M + H)	2.87
3370	 2CF ₃ CO ₂ H	422.2 (M + H)	2.79

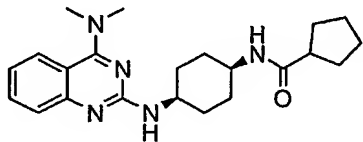
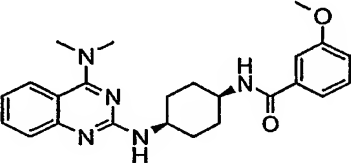
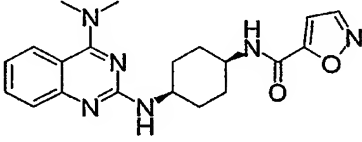
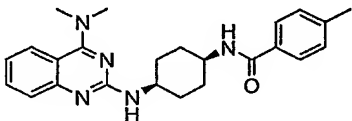
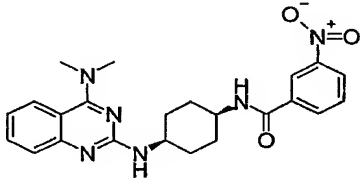
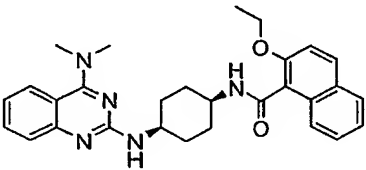
Example No:	Structure	ESI-MS	Retention Time (min)
3371	 $2\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	2.96
3372	 $3\text{CF}_3\text{CO}_2\text{H}$	427.2 (M + H)	2.53
3373	 $2\text{CF}_3\text{CO}_2\text{H}$	432.4 (M + H)	3.12
3374	 $3\text{CF}_3\text{CO}_2\text{H}$	447.4 (M + H)	2.45
3375	 $2\text{CF}_3\text{CO}_2\text{H}$	408.2 (M + H)	3.02
3376	 $2\text{CF}_3\text{CO}_2\text{H}$	496.4 (M + H)	2.81

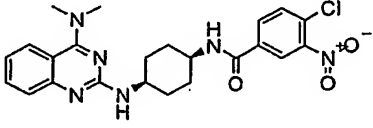
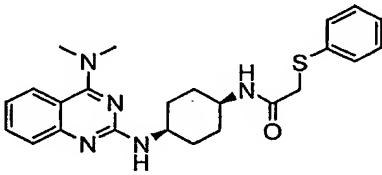
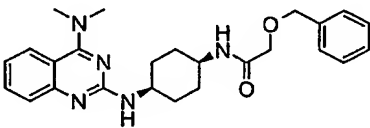
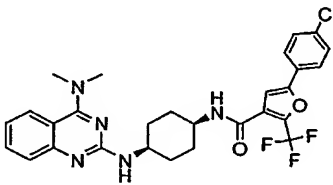
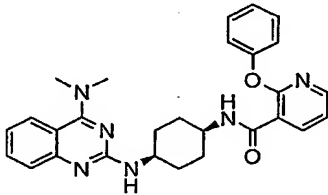
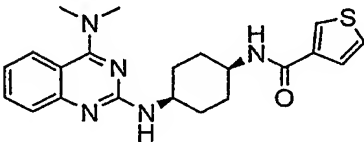
Example No.	Structure	ESI-MS	Rétention Time (min)
3377	 $2\text{CF}_3\text{CO}_2\text{H}$	400.2 (M + H)	2.81
3378	 $2\text{CF}_3\text{CO}_2\text{H}$	520.2 (M + H)	3.14
3379	 $2\text{CF}_3\text{CO}_2\text{H}$	410.4 (M + H)	3.12
3380	 $2\text{CF}_3\text{CO}_2\text{H}$	496.4 (M + H)	3.40
3381	 $2\text{CF}_3\text{CO}_2\text{H}$	496.4 (M + H)	3.17
3382	 $2\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	3.19

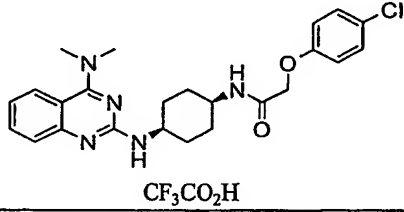
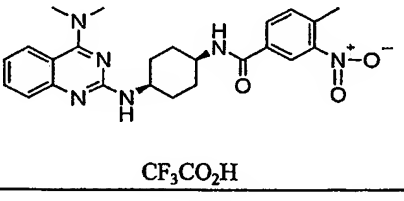
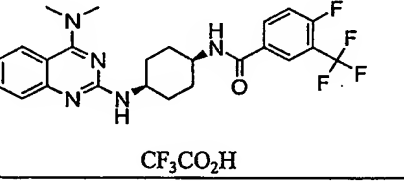
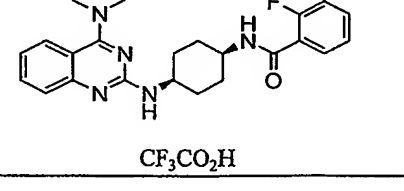
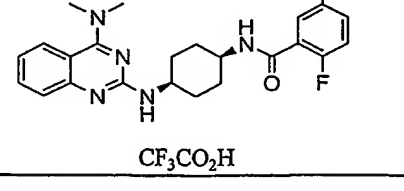
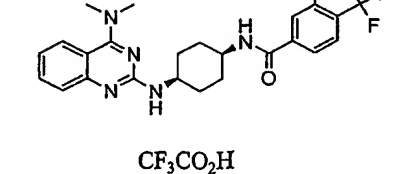
Example No.	Structure	ESI-MS	Retention Time (min)
3383	 $2\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	3.28
3384	 $2\text{CF}_3\text{CO}_2\text{H}$	440.4 (M + H)	2.74
3385	 $2\text{CF}_3\text{CO}_2\text{H}$	454.2 (M + H)	2.89
3386	 $2\text{CF}_3\text{CO}_2\text{H}$	404.4 (M + H)	3.09
3387	 $2\text{CF}_3\text{CO}_2\text{H}$	482.2 (M + H)	3.29
3388	 $3\text{CF}_3\text{CO}_2\text{H}$	458.4 (M + H)	2.99

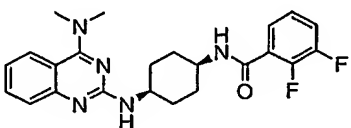
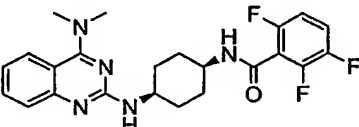
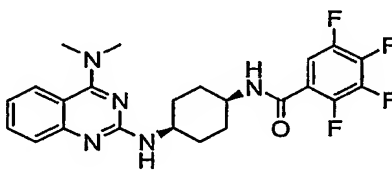
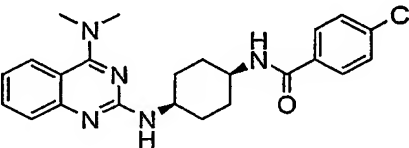
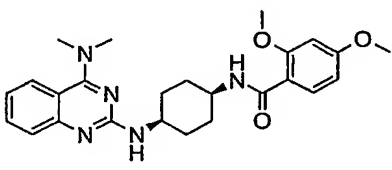
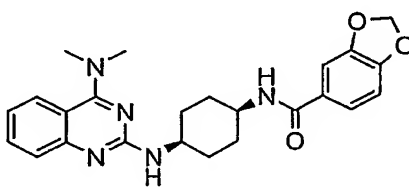
Example No.	Structure	ESI-MS	Retention Time (min)
3389	 $2\text{CF}_3\text{CO}_2\text{H}$	452.2 (M + H)	3.40
3390	 $2\text{CF}_3\text{CO}_2\text{H}$	560.2 (M + H)	3.73
3391	 $2\text{CF}_3\text{CO}_2\text{H}$	416.4 (M + H)	2.99
3392	 $2\text{CF}_3\text{CO}_2\text{H}$	518.6 (M + H)	4.08
3393	 $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	2.95
3394	 $\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	3.30

Example No.	Structure	ESI-MS	Retention Time (min)
3395	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3NC(=O)c4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.4 (M + H)	4.26
3396	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3NC(=O)c4cc(Cl)cc(Cl)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	4.39
3397	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3NC(=O)C(c1ccccc1)c2ccccc2</chem> $\text{CF}_3\text{CO}_2\text{H}$	480.4 (M + H)	4.37
3398	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3NC(=O)C(=O)c4cc(F)c(Cl)cc4N</chem> $\text{CF}_3\text{CO}_2\text{H}$	523.6 (M + H)	4.15
3399	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3NC(=O)c4cc(C)ccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	404.4 (M + H)	3.46
3400	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3NC(=O)c4cc(C)ccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	404.4 (M + H)	3.75

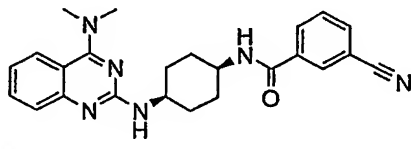
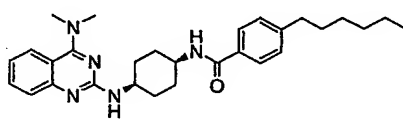
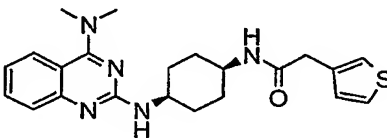
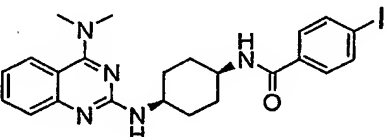
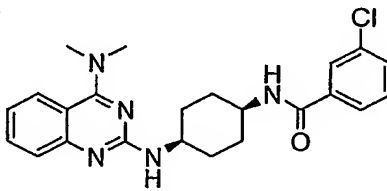
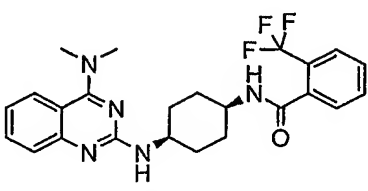
Example No.	Structure	ESI-MS	Retention Time (min)
3401	 <chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC(=C3)N[C@@H]4CCCC[C@H]4C(=O)N5CCCC5)C</chem> <chem>CC(F)(F)C(=O)O</chem>	382.4 (M + H)	3.65
3402	 <chem>COc1ccc(cc1)C(=O)N[C@@H]2CCCC[C@H]2N3C(=NC(=C3)N[C@@H]4CCCC[C@H]4C(=O)N5CCCC5)C</chem> <chem>CC(F)(F)C(=O)O</chem>	420.4 (M + H)	3.81
3403	 <chem>Cc1ccoc1C(=O)N[C@@H]2CCCC[C@H]2N3C(=NC(=C3)N[C@@H]4CCCC[C@H]4C(=O)N5CCCC5)C</chem> <chem>CC(F)(F)C(=O)O</chem>	381.2 (M + H)	3.33
3404	 <chem>CC1=CC=C(C=C1)C(=O)N[C@@H]2CCCC[C@H]2N3C(=NC(=C3)N[C@@H]4CCCC[C@H]4C(=O)N5CCCC5)C</chem> <chem>CC(F)(F)C(=O)O</chem>	404.4 (M + H)	3.93
3405	 <chem>[O-][N+](=O)c1ccc(cc1)C(=O)N[C@@H]2CCCC[C@H]2N3C(=NC(=C3)N[C@@H]4CCCC[C@H]4C(=O)N5CCCC5)C</chem> <chem>CC(F)(F)C(=O)O</chem>	435.2 (M + H)	3.40
3406	 <chem>COc1ccc2ccccc2c1C(=O)N[C@@H]3CCCC[C@H]3N4C(=NC(=C4)N[C@@H]5CCCC[C@H]5C(=O)N6CCCC6)C</chem> <chem>CC(F)(F)C(=O)O</chem>	484.4 (M + H)	4.15

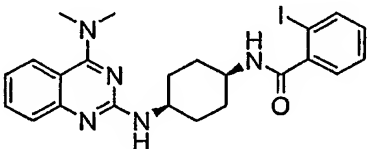
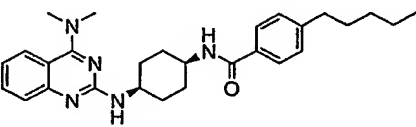
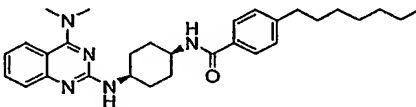
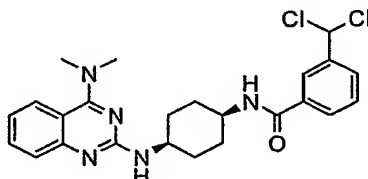
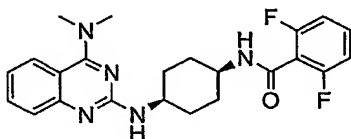
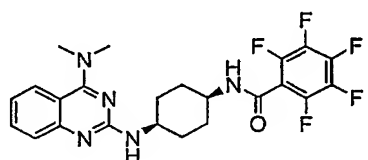
Example No.	Structure	ESI-MS	Retention Time (min)
3407	 <chem>CC1=NC2=CC=CC=C2N(C)C1N[C@H]3CCCC[C@H]3NC(=O)c4cc([N+](=O)[O-])cc(Cl)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	469.4 (M + H)	4.20
3408	 <chem>CC1=NC2=CC=CC=C2N(C)C1N[C@H]3CCCC[C@H]3NC(=O)CCSc4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	436.2 (M + H)	3.88
3409	 <chem>CC1=NC2=CC=CC=C2N(C)C1N[C@H]3CCCC[C@H]3NC(=O)COc4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	3.91
3410	 <chem>CC1=NC2=CC=CC=C2N(C)C1N[C@H]3CCCC[C@H]3NC(=O)C(F)(F)Fc4cc(Cl)ccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	558.4 (M + H)	4.92
3411	 <chem>CC1=NC2=CC=CC=C2N(C)C1N[C@H]3CCCC[C@H]3NC(=O)c4ccncc4Nc5ccccc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	483.4 (M + H)	4.08
3412	 <chem>CC1=NC2=CC=CC=C2N(C)C1N[C@H]3CCCC[C@H]3NC(=O)CCc4ccsc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	396.2 (M + H)	3.68

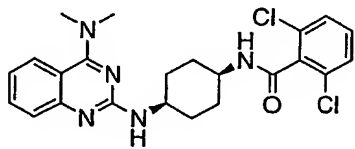
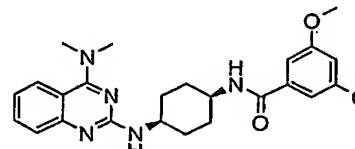
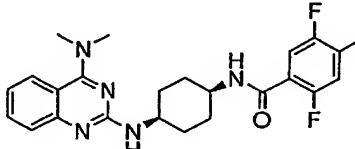
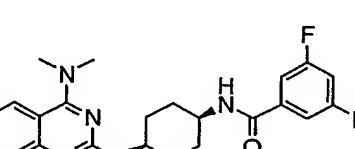
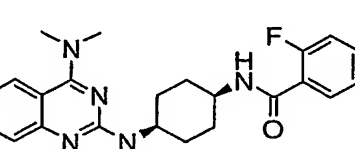
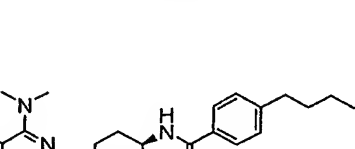
Example No.	Structure	ESI-MS	Retention Time (min)
3413	 <chem>CN(C)c1nc2c(ncn2C1N[C@H]3CCCC[C@H]3NC(=O)OCC4=CC=C(C=C4)Cl)C3=CC=CC=C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	454.2 (M + H)	3.70
3414	 <chem>CN(C)c1nc2c(ncn2C1N[C@H]3CCCC[C@H]3NC(=O)OC(=O)c4ccc(cc4)[N+](=O)[O-])C3=CC=CC=C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	449.4 (M + H)	4.09
3415	 <chem>CN(C)c1nc2c(ncn2C1N[C@H]3CCCC[C@H]3NC(=O)OC(=O)c4cc(F)c(C(F)(F)F)cc4)C3=CC=CC=C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	4.33
3416	 <chem>CN(C)c1nc2c(ncn2C1N[C@H]3CCCC[C@H]3NC(=O)OC(=O)c4cc(F)c(C(F)(F)F)c(F)c4)C3=CC=CC=C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.4 (M + H)	3.60
3417	 <chem>CN(C)c1nc2c(ncn2C1N[C@H]3CCCC[C@H]3NC(=O)OC(=O)c4cc(F)c(C(F)(F)F)cc4)C3=CC=CC=C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.4 (M + H)	4.23
3418	 <chem>CN(C)c1nc2c(ncn2C1N[C@H]3CCCC[C@H]3NC(=O)OC(=O)c4cc(F)c(C(F)(F)F)c(F)c4)C3=CC=CC=C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.4 (M + H)	4.38

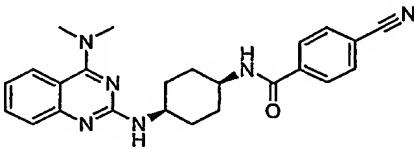
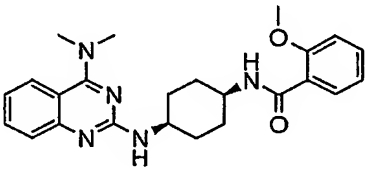
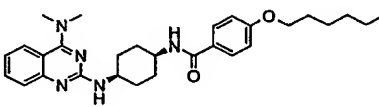
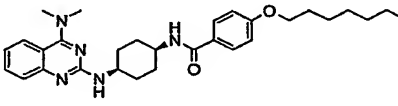
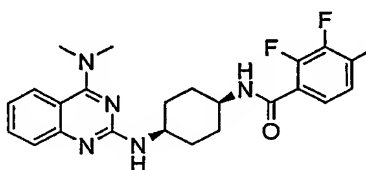
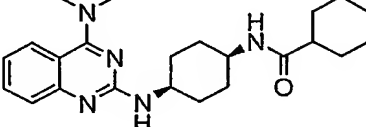
Example No.	Structure	ESI-MS	Retention Time (min)
3419	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N[C@H]3CCCC[C@H]3NC(=O)c4cc(F)c(F)c(F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	3.87
3420	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N[C@H]3CCCC[C@H]3NC(=O)c4cc(F)c(F)c(F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	444.4 (M + H)	3.86
3421	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N[C@H]3CCCC[C@H]3NC(=O)c4cc(F)c(F)c(F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	4.15
3422	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N[C@H]3CCCC[C@H]3NC(=O)c4ccc(Cl)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	4.06
3423	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N[C@H]3CCCC[C@H]3NC(=O)c4cc(OC)c(OC)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	4.03
3424	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N[C@H]3CCCC[C@H]3NC(=O)c4cc5c(c(c(OC5)O)O)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	434.2 (M + H)	3.75

Example No.	Structure	ESI-MS	Retention Time (min)
3425	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC(=O)c4cc(F)cc(F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	3.88
3426	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC(=O)c4cc(OC)c(OC)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	3.64
3427	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC(=O)c4cc(OC)c(OC)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	3.55
3428	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC(=O)c4ccc(CC)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	4.17
3429	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC(=O)c4ccc(OCC)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	4.03
3430	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC(=O)c4cc(Cl)c(Cl)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	4.45

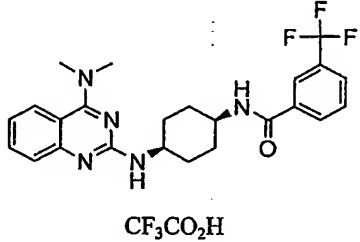
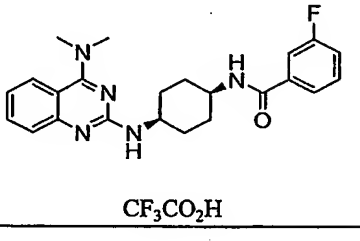
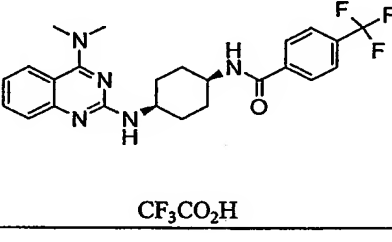
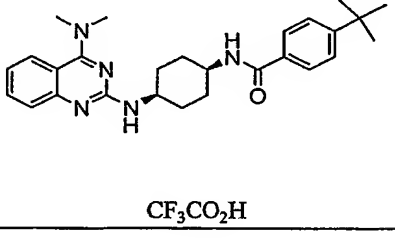
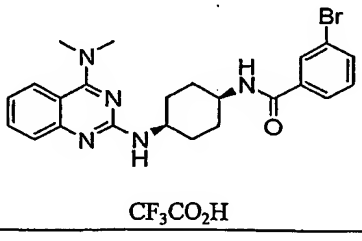
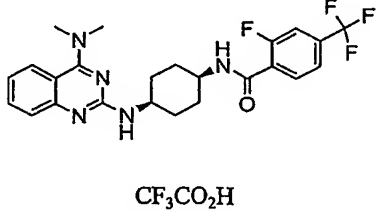
Example No.	Structure	ESI-MS	Retention Time (min)
3431	 CF ₃ CO ₂ H	415.4 (M + H)	3.76
3432	 CF ₃ CO ₂ H	474.4 (M + H)	5.06
3433	 CF ₃ CO ₂ H	410.2 (M + H)	3.64
3434	 CF ₃ CO ₂ H	516.2 (M + H)	4.24
3435	 CF ₃ CO ₂ H	424.2 (M + H)	4.09
3436	 CF ₃ CO ₂ H	458.2 (M + H)	3.89

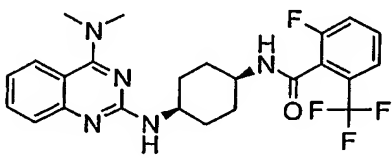
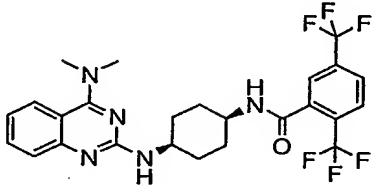
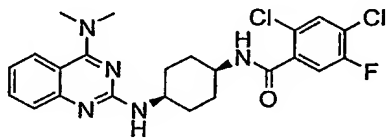
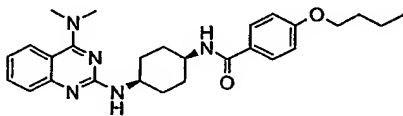
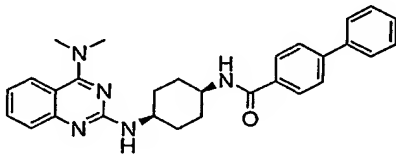
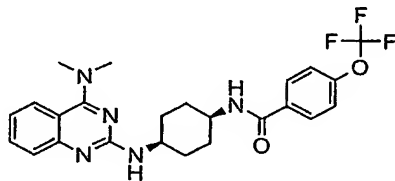
Example No.	Structure	ESI-MS	Retention Time (min)
3437	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3NC(=O)c4ccccc4I</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.2 (M + H)	3.88
3438	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3NC(=O)c4ccc(cc4)CCCC</chem> $\text{CF}_3\text{CO}_2\text{H}$	460.4 (M + H)	4.86
3439	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3NC(=O)c4ccc(cc4)CCCCC</chem> $\text{CF}_3\text{CO}_2\text{H}$	488.4 (M + H)	4.70
3440	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3NC(=O)c4ccc(cc4)C(Cl)Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.4 (M + H)	4.29
3441	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3NC(=O)c4cc(F)c(F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	3.69
3442	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3NC(=O)c4c(F)c(F)c(F)c4F</chem> $\text{CF}_3\text{CO}_2\text{H}$	480.2 (M + H)	4.16

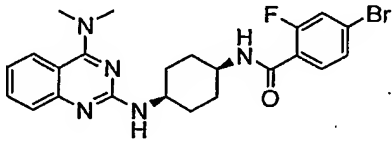
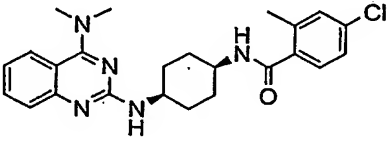
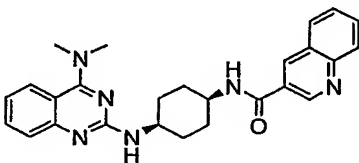
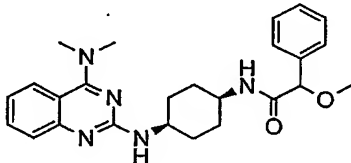
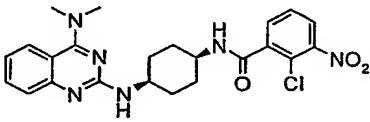
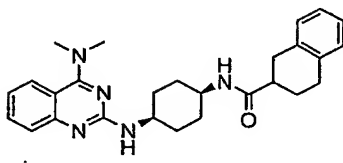
Example No.	Structure	ESI-MS	Retention Time (min)
3443	 <chem>CC1=NC2=CC=CC=C2N(C)C1N[C@H]3CCCC[C@H]3NC(=O)c1cc(Cl)cc(Cl)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	3.91
3444	 <chem>COc1cc(OC)cc(C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	3.95
3445	 <chem>Fc1cc(F)cc(C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C)cc1F</chem> $\text{CF}_3\text{CO}_2\text{H}$	444.4 (M + H)	4.01
3446	 <chem>Fc1cc(F)cc(C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	4.00
3447	 <chem>Fc1ccccc1C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	408.4 (M + H)	3.75
3448	 <chem>CCCC1=CC=C(C=C1)C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	446.6 (M + H)	4.65

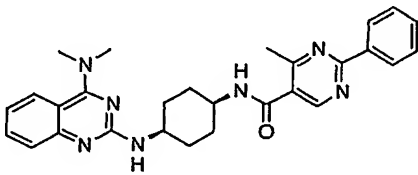
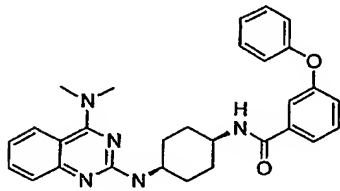
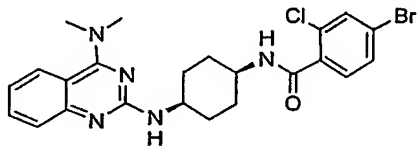
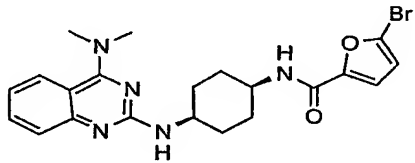
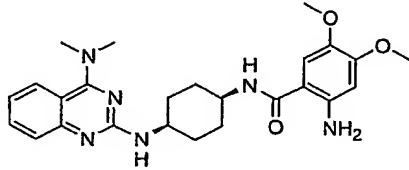
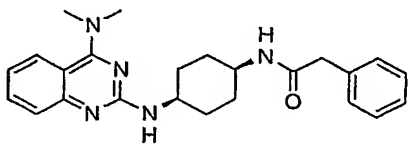
Example No.	Structure	ESI-MS	Retention Time (min)
3449	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N[C@H]3CCCC[C@H]3NC(=O)c4ccc(C#N)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	415.2 (M + H)	3.75
3450	 <chem>COc1ccccc1C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	3.91
3451	 <chem>CCOC1=CC=C(C=C1)C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	4.99
3452	 <chem>CCOC1=CC=C(C=C1)C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	504.4 (M + H)	5.16
3453	 <chem>Fc1cc(F)c(C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C)cc1F</chem> $\text{CF}_3\text{CO}_2\text{H}$	444.4 (M + H)	4.00
3454	 <chem>C1CCCCC1C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	396.2 (M + H)	3.85

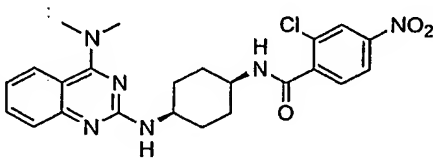
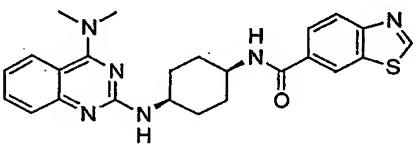
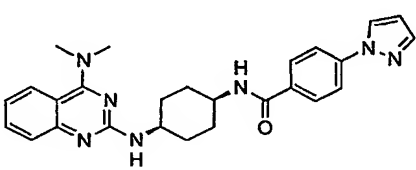
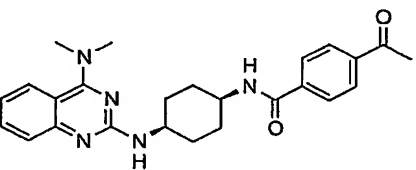
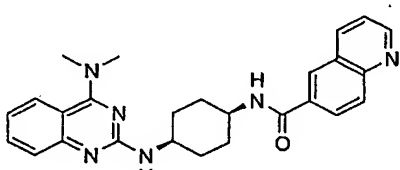
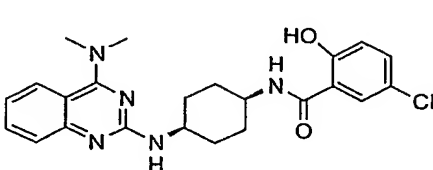
Example No.	Structure	ESI-MS	Retention Time (min)
3455	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c4cc(F)c(F)c(F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	526.6 (M + H)	4.69
3456	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c4ccc(F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	408.4 (M + H)	3.30
3457	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c4cc(OC)c(OC)c(OC)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	480.4 (M + H)	3.76
3458	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c4cc(F)c(F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	3.86
3459	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c4ccccc4Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	3.76
3460	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c4c5ccccc5c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.4 (M + H)	4.05

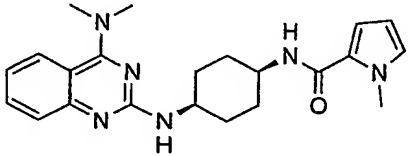
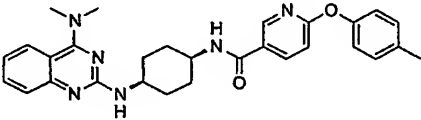
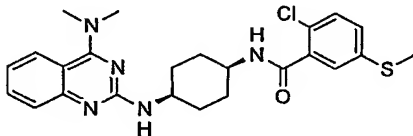
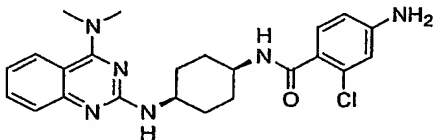
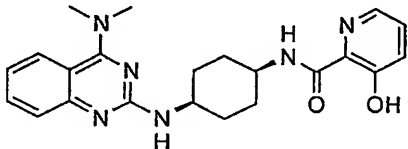
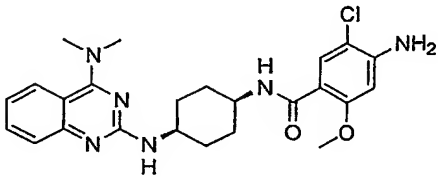
Example No.	Structure	ESI-MS	Retention Time (min)
3461	 CF ₃ CO ₂ H	458.4 (M + H)	4.25
3462	 CF ₃ CO ₂ H	408.2 (M + H)	3.84
3463	 CF ₃ CO ₂ H	458.2 (M + H)	4.25
3464	 CF ₃ CO ₂ H	446.6 (M + H)	4.44
3465	 CF ₃ CO ₂ H	470.2 (M + H)	4.13
3466	 CF ₃ CO ₂ H	476.2 (M + H)	4.25

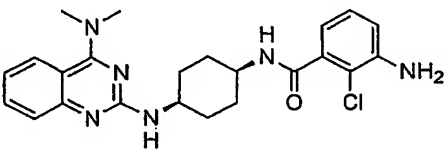
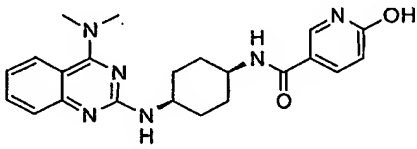
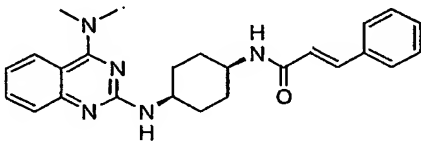
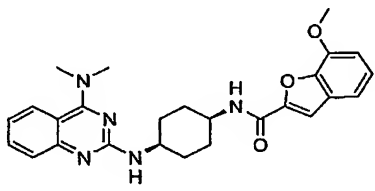
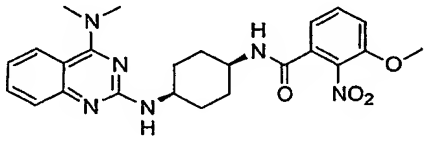
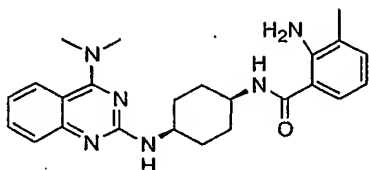
Example No.	Structure	ESI-MS	Retention Time (min)
3467	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3NC(=O)c1cc(F)c(F)c(F)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	3.92
3468	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3NC(=O)c1cc(F)c(F)c(F)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	526.4 (M + H)	4.31
3469	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3NC(=O)c1cc(Cl)c(F)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	4.15
3470	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3NC(=O)c1ccc(OCC)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	4.48
3471	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3NC(=O)c1ccc(cc1)-c2ccccc2</chem> $\text{CF}_3\text{CO}_2\text{H}$	466.4 (M + H)	4.45
3472	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3NC(=O)c1ccc(OC(F)(F)F)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	4.29

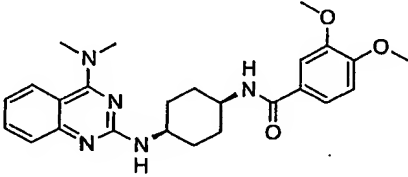
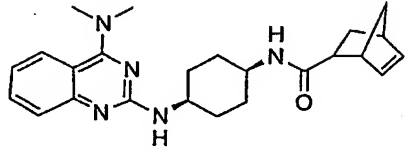
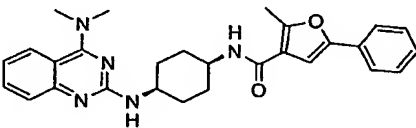
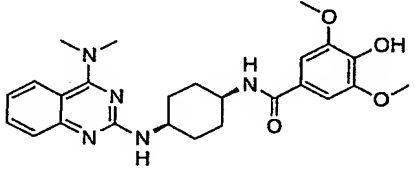
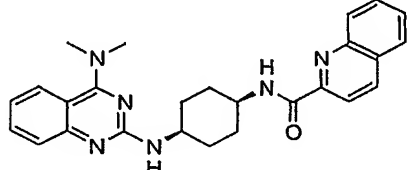
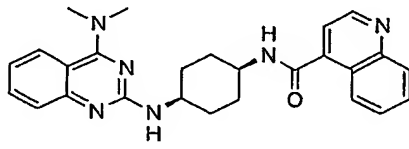
Example No.	Structure	ESI-MS	Retention Time (min)
3473	 $\text{CF}_3\text{CO}_2\text{H}$	486.2 (M + H)	4.32
3474	 $\text{CF}_3\text{CO}_2\text{H}$	438.4 (M + H)	4.31
3475	 $2\text{CF}_3\text{CO}_2\text{H}$	441.4 (M + H)	3.75
3476	 $\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	4.10
3477	 $\text{CF}_3\text{CO}_2\text{H}$	469.4 (M + H)	4.19
3478	 $\text{CF}_3\text{CO}_2\text{H}$	444.4 (M + H)	4.36

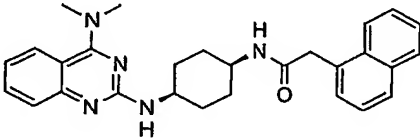
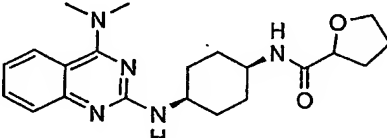
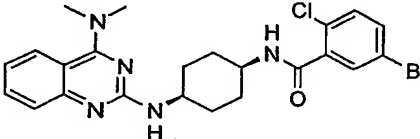
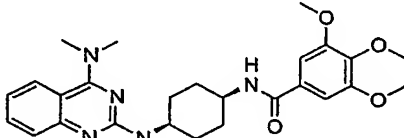
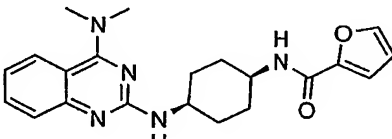
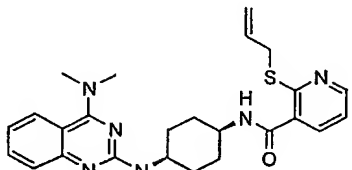
Example No.	Structure	ESI-MS	Retention Time (min)
3479	 $3\text{CF}_3\text{CO}_2\text{H}$	482.4 (M + H)	4.35
3480	 $\text{CF}_3\text{CO}_2\text{H}$	482.4 (M + H)	4.64
3481	 $\text{CF}_3\text{CO}_2\text{H}$	502.2 (M + H)	4.37
3482	 $\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	4.08
3483	 $2\text{CF}_3\text{CO}_2\text{H}$	465.4 (M + H)	3.66
3484	 $\text{CF}_3\text{CO}_2\text{H}$	404.4 (M + H)	4.03

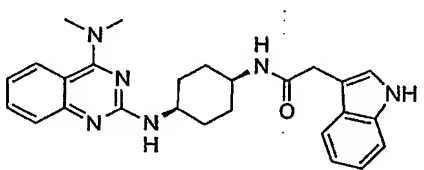
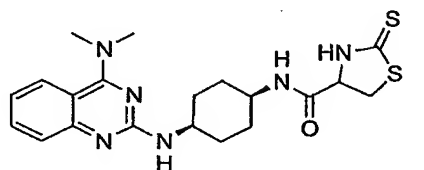
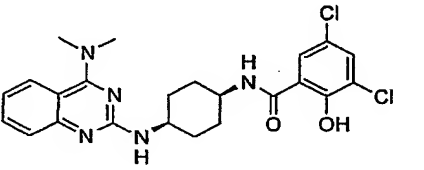
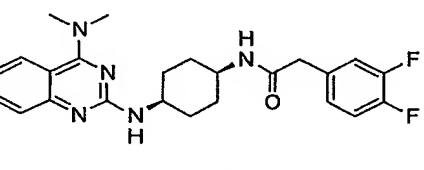
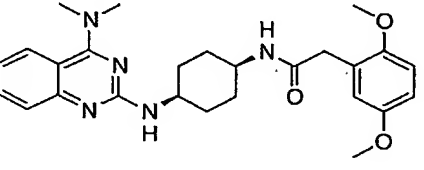
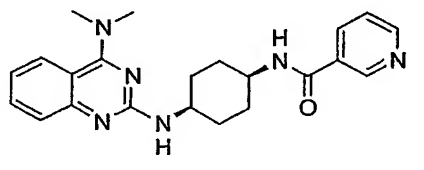
Example No.	Structure	ESI-MS	Retention Time (min)
3485	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N(C)C(C1)N3CCCCC3NC(=O)c4cc([N+](=O)[O-])cc(Cl)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	469.4 (M + H)	4.23
3486	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N(C)C(C1)N3CCCCC3NC(=O)c4ccc5c(s4)nn5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	447.4 (M + H)	3.94
3487	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N(C)C(C1)N3CCCCC3NC(=O)c4ccc5c(n4)cnc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	456.2 (M + H)	4.07
3488	 <chem>CC(=O)c1ccc(cc1)NC(=O)N2CCCCC2N3C(=N)N(C)C(C3)N4=CC=CC=C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	432.4 (M + H)	3.99
3489	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N(C)C(C1)N3CCCCC3NC(=O)c4ccc5c6ccncc6cc5n4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	441.3 (M + H)	1.70
3490	 <chem>Oc1cc(Cl)ccc1NC(=O)N2CCCCC2N3C(=N)N(C)C(C3)N4=CC=CC=C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.2 (M + H)	4.57

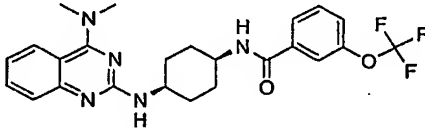
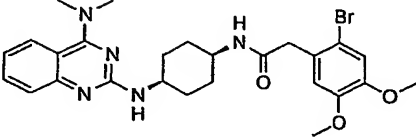
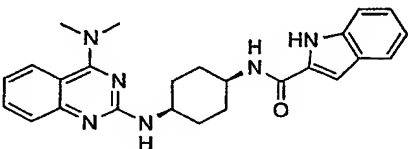
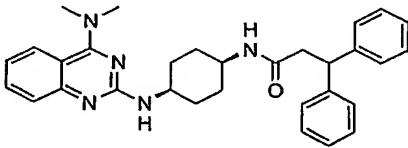
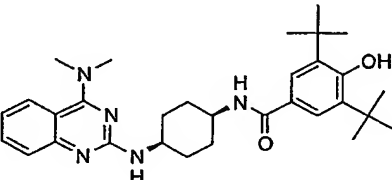
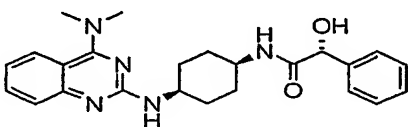
Example No.	Structure	ESI-MS	Retention Time (min)
3491	 $2\text{CF}_3\text{CO}_2\text{H}$	393.4 (M + H)	4.01
3492	 $2\text{CF}_3\text{CO}_2\text{H}$	497.4 (M + H)	4.45
3493	 $\text{CF}_3\text{CO}_2\text{H}$	470.2 (M + H)	2.40
3494	 $2\text{CF}_3\text{CO}_2\text{H}$	439.4 (M + H)	1.92
3495	 $2\text{CF}_3\text{CO}_2\text{H}$	407.4 (M + H)	2.30
3496	 $2\text{CF}_3\text{CO}_2\text{H}$	469.5 (M + H)	2.27

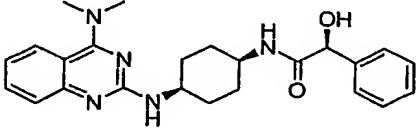
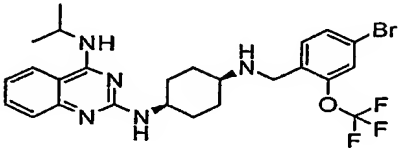
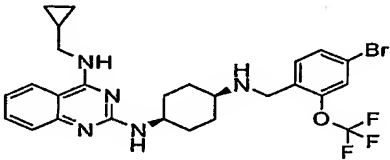
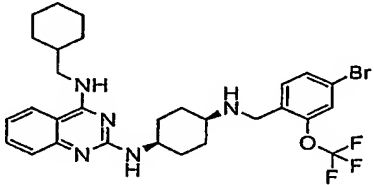
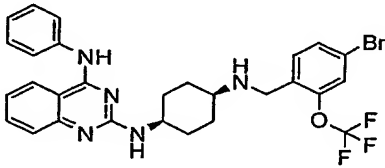
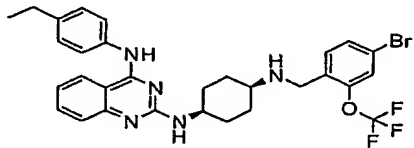
Example No.	Structure	ESI-MS	Retention Time (min)
3497	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC(=O)c4cc(N)cc(Cl)c4)c5ccccc15</chem> $2\text{CF}_3\text{CO}_2\text{H}$	439.4 (M + H)	1.93
3498	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC(=O)c4cc(O)cn4)c5ccccc15</chem> $2\text{CF}_3\text{CO}_2\text{H}$	407.4 (M + H)	1.62
3499	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC(=O)/C=C/c4ccccc4)c5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	416.3 (M + H)	2.34
3500	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC(=O)c4c5cc(OC)ccc5oc4)c6ccccc16</chem> $\text{CF}_3\text{CO}_2\text{H}$	460.4 (M + H)	2.46
3501	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC(=O)c4cc(OC)cc([N+](=O)[O-])c4)c5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	465.4 (M + H)	4.13
3502	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC(=O)c4cc(C)cc(N)c4)c5ccccc15</chem> $2\text{CF}_3\text{CO}_2\text{H}$	419.4 (M + H)	3.87

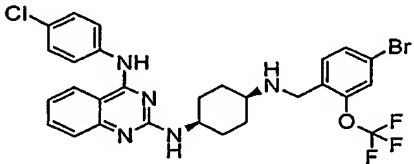
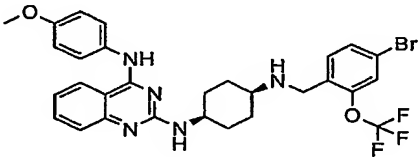
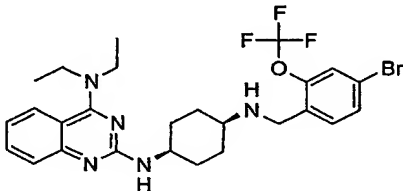
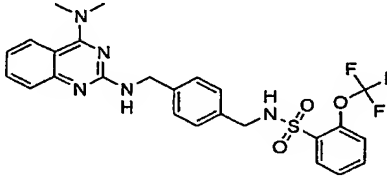
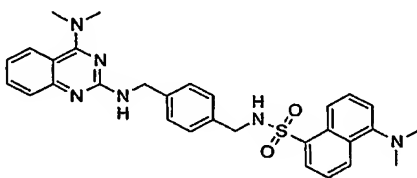
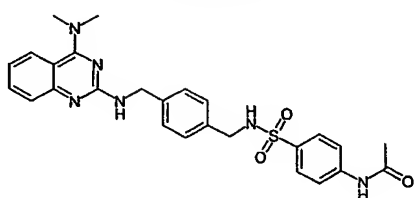
Example No.	Structure	ESI-MS	Retention Time (min)
3503	 <chem>COc1ccc(cc1)C(=O)N[C@H]2CCCC[C@H]2Nc3nc(C)c(C)n3</chem> $\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	3.97
3504	 <chem>C1=CC2=C(C1)C=CC2C(=O)N[C@H]3CCCC[C@H]3Nc4nc(C)c(C)n4</chem> $\text{CF}_3\text{CO}_2\text{H}$	406.2 (M + H)	2.18
3505	 <chem>Cc1cc(ccc1n1ccoc1)C(=O)N[C@H]2CCCC[C@H]2Nc3nc(C)c(C)n3</chem> $\text{CF}_3\text{CO}_2\text{H}$	470.4 (M + H)	4.74
3506	 <chem>COc1cc(O)cc(OC)c1C(=O)N[C@H]2CCCC[C@H]2Nc3nc(C)c(C)n3</chem> $\text{CF}_3\text{CO}_2\text{H}$	466.4 (M + H)	3.83
3507	 <chem>c1ccc2nc3ccccc3cc2n1C(=O)N[C@H]4CCCC[C@H]4Nc5nc(C)c(C)n5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	441.2 (M + H)	4.38
3508	 <chem>c1ccc2nc3ccccc3cc2n1C(=O)N[C@H]4CCCC[C@H]4Nc5nc(C)c(C)n5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	441.2 (M + H)	3.62

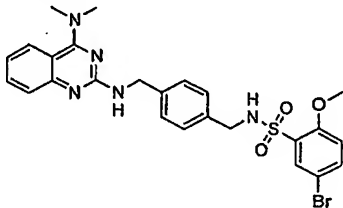
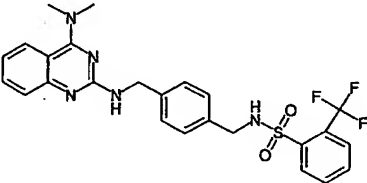
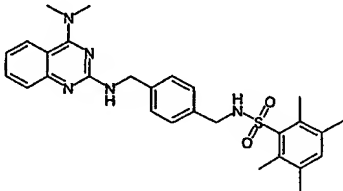
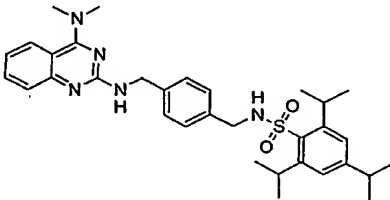
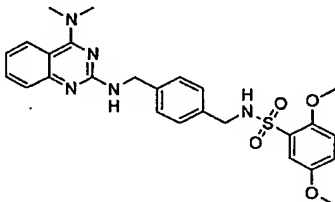
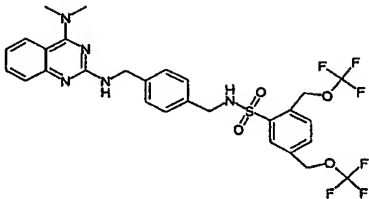
Example No.	Structure	ESI-MS	Retention Time (min)
3509	 $\text{CF}_3\text{CO}_2\text{H}$	454.5 (M + H)	2.44
3510	 $\text{CF}_3\text{CO}_2\text{H}$	384.4 (M + H)	3.67
3511	 $\text{CF}_3\text{CO}_2\text{H}$	502.2 (M + H)	4.37
3512	 $\text{CF}_3\text{CO}_2\text{H}$	480.5 (M + H)	2.18
3513	 $\text{CF}_3\text{CO}_2\text{H}$	380.2 (M + H)	3.81
3514	 $2\text{CF}_3\text{CO}_2\text{H}$	463.2 (M + H)	4.23

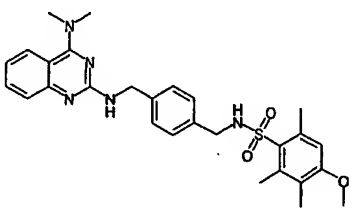
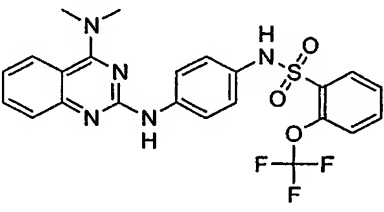
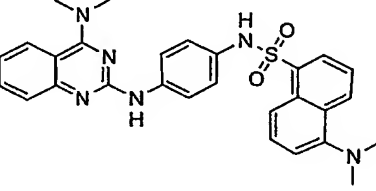
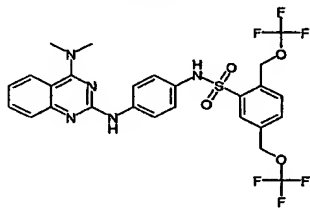
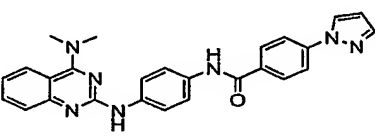
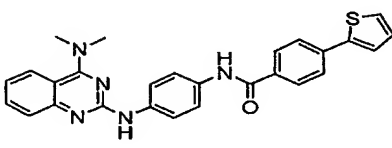
Example No.	Structure	ESI-MS	Retention Time (min)
3515	 <chem>CN(C)c1nc2c(ncn2c1)N[C@H]3CCCC[C@H]3NC(=O)Cc4c[nH]c5ccccc45</chem> $2\text{CF}_3\text{CO}_2\text{H}$	443.4 (M + H)	2.12
3516	 <chem>CN(C)c1nc2c(ncn2c1)N[C@H]3CCCC[C@H]3NC(=O)C4SCC(S)N4</chem> $\text{CF}_3\text{CO}_2\text{H}$	431.1 (M + H)	1.90
3517	 <chem>CN(C)c1nc2c(ncn2c1)N[C@H]3CCCC[C@H]3NC(=O)c4cc(Cl)c(Cl)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	5.05
3518	 <chem>CN(C)c1nc2c(ncn2c1)N[C@H]3CCCC[C@H]3NC(=O)Cc4cc(F)c(F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.5 (M + H)	2.33
3519	 <chem>CN(C)c1nc2c(ncn2c1)N[C@H]3CCCC[C@H]3NC(=O)Cc4cc(OC)c(OC)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	464.5 (M + H)	2.20
3520	 <chem>CN(C)c1nc2c(ncn2c1)N[C@H]3CCCC[C@H]3NC(=O)c4ccncc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	391.1 (M + H)	1.59

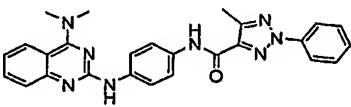
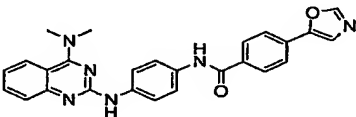
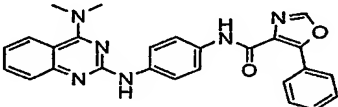
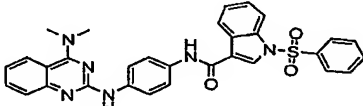
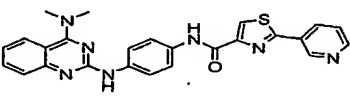
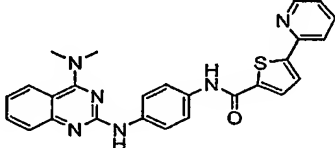
Example No.	Structure	ESI-MS	Retention Time (min)
3521	 $\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	4.53
3522	 $\text{CF}_3\text{CO}_2\text{H}$	542.2 (M + H)	2.26
3523	 $2\text{CF}_3\text{CO}_2\text{H}$	429.3 (M + H)	2.41
3524	 $\text{CF}_3\text{CO}_2\text{H}$	494.6 (M + H)	2.59
3525	 $\text{CF}_3\text{CO}_2\text{H}$	518.5 (M + H)	2.96
3526	 $\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.19

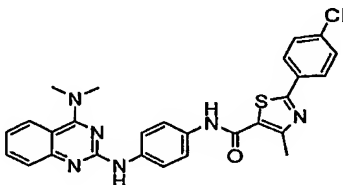
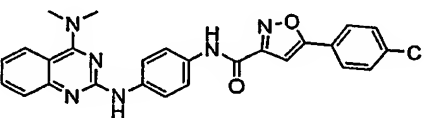
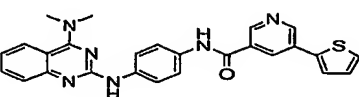
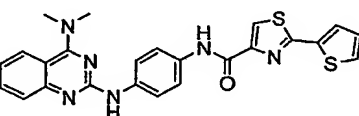
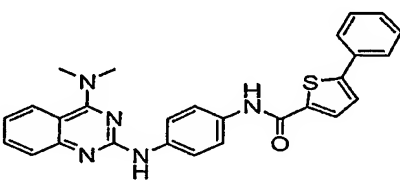
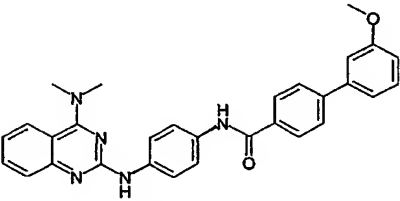
Example No.	Structure	ESI-MS	Retention Time (min)
3527	 <p style="text-align: center;">$\text{CF}_3\text{CO}_2\text{H}$</p>	420.4 (M + H)	2.19
3528	 <p style="text-align: center;">$2\text{CF}_3\text{CO}_2\text{H}$</p>	552.0 (M + H)	2.45
3529	 <p style="text-align: center;">$2\text{CF}_3\text{CO}_2\text{H}$</p>	564.2 (M + H)	2.48
3530	 <p style="text-align: center;">$2\text{CF}_3\text{CO}_2\text{H}$</p>	606.0 (M + H)	2.86
3531	 <p style="text-align: center;">$2\text{CF}_3\text{CO}_2\text{H}$</p>	586.2 (M + H)	3.20
3532	 <p style="text-align: center;">$2\text{CF}_3\text{CO}_2\text{H}$</p>	614.4 (M + H)	2.76

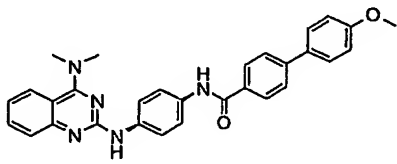
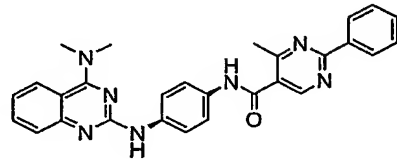
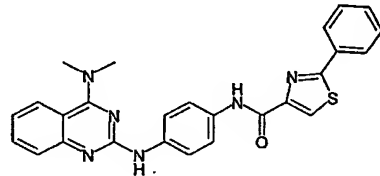
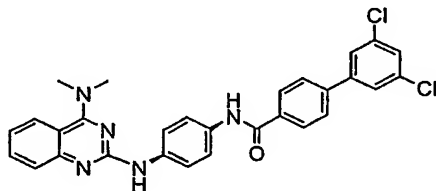
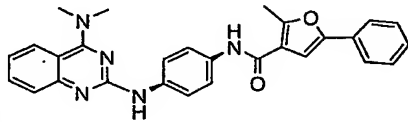
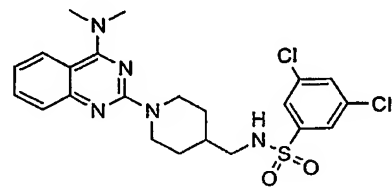
Example No.	Structure	ESI-MS	Retention Time (min)
3533	 $2\text{CF}_3\text{CO}_2\text{H}$	620.0 (M + H)	2.68
3534	 $2\text{CF}_3\text{CO}_2\text{H}$	616.0 (M + H)	2.56
3535	 $2\text{CF}_3\text{CO}_2\text{H}$	566.0 (M + H)	2.54
3536	 $\text{CF}_3\text{CO}_2\text{H}$	532.2 (M + H)	3.35
3537	 $2\text{CF}_3\text{CO}_2\text{H}$	541.4 (M + H)	3.11
3538	 $\text{CF}_3\text{CO}_2\text{H}$	505.2 (M + H)	2.98

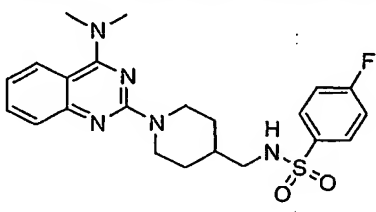
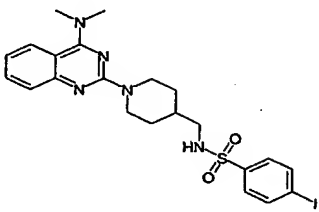
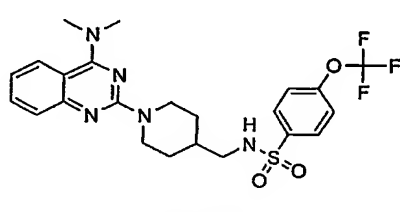
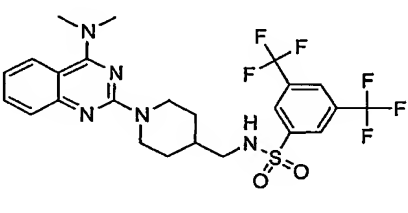
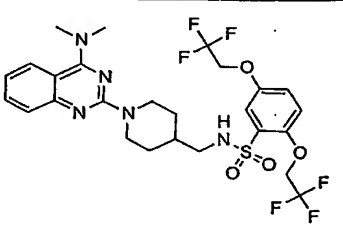
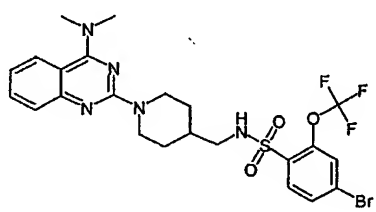
Example No.	Structure	ESI-MS	Retention Time (min)
3539	 <chem>COc1cc(Br)cc(S(=O)(=O)Nc2ccc(CN3C=NC4=CC=CC=C4N3C)cc2)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	556 (M + H)	3.37
3540	 <chem>FC1(F)C2=CC=CC=C2S(=O)(=O)Nc3ccc(CN4C=NC5=CC=CC=C4N5C)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.4 (M + H)	3.39
3541	 <chem>CC1=C(C)C=C(C)S(=O)(=O)Nc2ccc(CN3C=NC4=CC=CC=C4N3C)cc2</chem> $\text{CF}_3\text{CO}_2\text{H}$	504.4 (M + H)	3.61
3542	 <chem>CC1=C(C)C=C(C)S(=O)(=O)Nc2ccc(CN3C=NC4=CC=CC=C4N3C)cc2</chem> $\text{CF}_3\text{CO}_2\text{H}$	574.4 (M + H)	4.27
3543	 <chem>COc1cc(OC)cc(S(=O)(=O)Nc2ccc(CN3C=NC4=CC=CC=C4N3C)cc2)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	508.2 (M + H)	3.17
3544	 <chem>COc1cc(CF3)cc(S(=O)(=O)Nc2ccc(CN3C=NC4=CC=CC=C4N3C)cc2)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	644.2 (M + H)	3.63

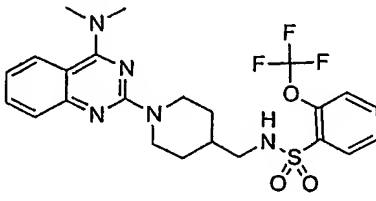
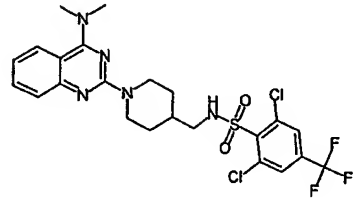
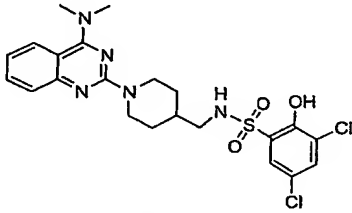
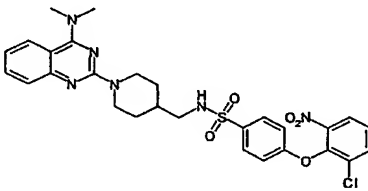
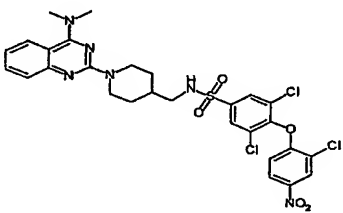
Example No.	Structure	ESI-MS	Retention Time (min)
3545	 <chem>CC1=NC2=CC=CC=C2N(C)N=C1NC3=CC=C(CS(=O)(=O)C4=CC(OC)=C(OC)C4)C=C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	520.4 (M + H)	3.56
3546	 <chem>CC1=NC2=CC=CC=C2N(C)N=C1NC3=CC=C(NC(=O)S(=O)(=O)C4=CC(OC(F)(F)F)=CC=C4)C=C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	504.2 (M + H)	3.25
3547	 <chem>CC1=NC2=CC=CC=C2N(C)N=C1NC3=CC=C(NC(=O)S(=O)(=O)C4=CC=C(NC)C=C5C=CC=CC=C45)C=C3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	513.4 (M + H)	2.86
3548	 <chem>CC1=NC2=CC=CC=C2N(C)N=C1NC3=CC=C(NS(=O)(=O)C4=CC(OC(F)(F)F)=CC(OC(F)(F)F)=C4)C=C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	616.2 (M + H)	3.73
3549	 <chem>CC1=NC2=CC=CC=C2N(C)N=C1NC3=CC=C(NC(=O)C4=CC=C(C=C4)C5=CN=CN5)C=C3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	2.79
3550	 <chem>CC1=NC2=CC=CC=C2N(C)N=C1NC3=CC=C(NC(=O)C4=CC=C(C=C4)C5=CC=C(S)C=C5)C=C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	466.2 (M + H)	3.35

Example No.	Structure	ESI-MS	Retention Time (min)
3551	 $2\text{CF}_3\text{CO}_2\text{H}$	465.2 (M + H)	3.34
3552	 $\text{CF}_3\text{CO}_2\text{H}$	451.2 (M + H)	3.83
3553	 $\text{CF}_3\text{CO}_2\text{H}$	451.2 (M + H)	4.10
3554	 $\text{CF}_3\text{CO}_2\text{H}$	563.2 (M + H)	4.33
3555	 $2\text{CF}_3\text{CO}_2\text{H}$	468.4 (M + H)	3.66
3556	 $2\text{CF}_3\text{CO}_2\text{H}$	467.4 (M + H)	2.85

Example No.	Structure	ESI-MS	Retention Time (min)
3557	 $\text{CF}_3\text{CO}_2\text{H}$	515.4 (M + H)	3.52
3558	 $\text{CF}_3\text{CO}_2\text{H}$	485.2 (M + H)	3.40
3559	 $2\text{CF}_3\text{CO}_2\text{H}$	467.4 (M + H)	3.90
3560	 $\text{CF}_3\text{CO}_2\text{H}$	473.4 (M + H)	4.17
3561	 $\text{CF}_3\text{CO}_2\text{H}$	467.4 (M + H)	3.57
3562	 $\text{CF}_3\text{CO}_2\text{H}$	490.2 (M + H)	4.00

Example No.	Structure	ESI-MS	Retention Time (min)
3563	 <chem>COc1ccc(cc1)C(=O)Nc2ccc(cc2)Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	490.2 (M + H)	3.99
3564	 <chem>c1ccc(cc1)c2nc3ccccc3n2C(=O)Nc4ccc(cc4)Nc5nc6ccccc6n5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	3.76
3565	 <chem>c1ccc(cc1)c2sc(C(=O)Nc3ccc(cc3)Nc4nc5ccccc5n4)nc2</chem> $\text{CF}_3\text{CO}_2\text{H}$	467.2 (M + H)	4.07
3566	 <chem>Clc1cc(Cl)ccc1C(=O)Nc2ccc(cc2)Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	528.2 (M + H)	4.53
3567	 <chem>c1ccc(cc1)c2oc(C(=O)Nc3ccc(cc3)Nc4nc5ccccc5n4)c(C)c2</chem> $\text{CF}_3\text{CO}_2\text{H}$	464.2 (M + H)	4.11
3568	 <chem>Clc1cc(Cl)ccc1S(=O)(=O)NCC2CCN(C2)c3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	494.0 (M + H)	3.43

Example No.	Structure	ESI-MS	Retention Time (min)
3569	 <chem>CC1=NC2=C(N1)N=CN=C2CN3CCCCC3CNS(=O)(=O)c4ccc(F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	444.0 (M + H)	3.03
3570	 <chem>CC1=NC2=C(N1)N=CN=C2CN3CCCCC3CNS(=O)(=O)c4ccc(I)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	552.0 (M + H)	3.30
3571	 <chem>CC1=NC2=C(N1)N=CN=C2CN3CCCCC3CNS(=O)(=O)c4ccc(OC(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	510.0 (M + H)	3.37
3572	 <chem>CC1=NC2=C(N1)N=CN=C2CN3CCCCC3CNS(=O)(=O)c4cc(C(F)(F)F)c(C(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	562.0 (M + H)	3.66
3573	 <chem>CC1=NC2=C(N1)N=CN=C2CN3CCCCC3CNS(=O)(=O)c4cc(OC(F)(F)F)cc(OC(F)(F)F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	622.0 (M + H)	3.61
3574	 <chem>CC1=NC2=C(N1)N=CN=C2CN3CCCCC3CNS(=O)(=O)c4cc(Br)cc(OC(F)(F)F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	588.0 (M + H)	3.59

Example No.	Structure	ESI-MS	Retention Time (min)
3575	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCN(CCC3S(=O)(=O)C4=CC=CC=C4OC5C=CC=C(C5)C(F)(F)F)C4C(=O)O</chem> $\text{CF}_3\text{CO}_2\text{H}$	510.0 (M + H)	3.31
3576	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCN(CCC3S(=O)(=O)C4=CC=C(C=C4)C(F)(F)F)C5=CC=C(C=C5)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	562.0 (M + H)	3.61
3577	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCN(CCC3S(=O)(=O)C4=CC=C(C=C4)O)C5=CC=C(C=C5)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	510.0 (M + H)	3.35
3578	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCN(CCC3S(=O)(=O)C4=CC=C(C=C4)O)C5=CC=C(C=C5)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	597.0 (M + H)	3.55
3579	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCN(CCC3S(=O)(=O)C4=CC=C(C=C4)O)C5=CC=C(C=C5)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	665.0 (M + H)	4.02

Assay Procedures

Compounds identified and disclosed throughout this patent document were assayed according to the protocols found in co-pending patent application having U.S. Serial Number 09/826,509, which is incorporated herein by reference.

Example 3580

Preparation of Endogenous MCH Receptor.

The endogenous human MCH receptor was obtained by PCR using genomic DNA as template and rTth polymerase (Perkin Elmer) with the buffer system provided by the manufacturer, 0.25 μ M of each primer, and 0.2 mM of each 4 nucleotides. The cycle condition was 30 cycles of 94°C for 1 min, 56°C for 1min and 72 °C for 1 min and 20 sec. The 5' PCR primer contained a HindIII site with the sequence:

5'-GTGAAGCTTGCCTCTGGTGCCTGCAGGAGG-3' (SEQ.ID.NO.:1)

and the 3' primer contained an EcoRI site with the sequence:

5'-GCAGAATTCCCGGTGGCGTGTGTGGTGCCC-3' (SEQ.ID.NO.:2).

The 1.3 kb PCR fragment was digested with HindIII and EcoRI and cloned into HindIII-EcoRI site of CMVp expression vector. Later the cloning work by Lakaye et al showed that there is an intron the coding region of the gene. Thus the 5' end of the cDNA was obtained by 5' RACE PCR using Clontech's marathon-ready hypothalamus cDNA as template and the manufacturer's recommended protocol for cycling condition. The 5' RACE PCR for the first and second round PCR were as follows:

5'-CATGAGCTGGTGGATCATGAAGGG-3' (SEQ.ID.NO.:3) and

5'-ATGAAGGGCATGCCAGGAGAAAG-3' (SEQ.ID.NO.:4).

Nucleic acid and amino acid sequences were thereafter determined and verified with the published sequences found on GenBank having Accession Number U71092.

Example 3581

Preparation of Non-Endogenous, Constitutively Active MCH Receptor.

Preparation of a non-endogenous version of the human MCH receptor was accomplished by creating a MCH-IC3-SST2 mutation (*see*; SEQ.ID.NO.:7 for nucleic acid sequence, and SEQ.ID.NO.:8 for amino acid sequence). Blast result showed that MCH receptor had the highest sequence homology to known SST2 receptor. Thus the third intracellular loop ("IC3") of MCH receptor was replaced with that of the IC3 of SST2

receptor to see if the chimera would show constitutive activity.

The BamHI-BstEII fragment containing IC3 of MCH receptor was replaced with synthetic oligonucleotides that contained the IC3 of SST2. The PCR sense mutagenesis primer used had the following sequence:

5'-GATCCTGCAGAAGGTGAAGTCCTCTGGAATCCGAGTGGGCTCCTCTAAGAG
GAAGAAGTCTGAGAAGAAG-3' (SEQ.ID.NO.:9)

and the antisense primer had the following sequence:

5'-GTGACCTTCTTCTCAGACTTCTTCTCTTAGAGGAGCCCACTCGGATTCCAG
AGGACTTCACCTTCTGCAG-3' (SEQ.ID.NO.:10).

The endogenous MCH receptor cDNA was used as a template.

Example 3582

GPCR Fusion Protein Preparation.

MCH Receptor-Gi α Fusion Protein construct was made as follows: primers were designed for endogenous MCH receptor was as follows:

5'-GTGAAGCTTGCCCGGGCAGGATGGACCTGG-3' (SEQ.ID.NO.:11; sense)

5'-ATCTAGAGGTGCCTTTGCTTTCTG-3' (SEQ.ID.NO.:12; antisense).

The sense and anti-sense primers included the restriction sites for KB4 and XbaI, respectively.

PCR was utilized to secure the respective receptor sequences for fusion within the Gi α universal vector disclosed above, using the following protocol for each: 100ng cDNA for MCH receptor was added to separate tubes containing 2ul of each primer (sense and anti-sense), 3uL of 10mM dNTPs, 10uL of 10XTaqPlus™ Precision buffer, 1uL of TaqPlus™ Precision polymerase (Stratagene: #600211), and 80uL of water. Reaction temperatures and cycle times for MCH receptor were as follows: the initial denaturing step was done at 94°C for five minutes, and a cycle of 94°C for 30 seconds; 55°C for 30 seconds; 72°C for two minutes. A final extension time was done at 72°C for ten minutes. PCR product was run on a 1% agarose gel and then purified (data not shown). The purified product was digested with KB4 and XbaI (New England Biolabs) and the desired inserts will be isolated, purified and ligated into the Gi universal vector at the respective restriction site. The positive clones were isolated following transformation and determined by restriction enzyme digest; expression using 293 cells was accomplished

following the protocol set forth *infra*. Each positive clone for MCH receptor: Gi-Fusion Protein was sequenced and made available for the direct identification of candidate compounds. (See, SEQ.ID.NO.:13 for nucleic acid sequence and SEQ.ID.NO.:14 for amino acid sequence).

Endogenous version of MCH receptor was fused upstream from the G protein Gi and is located at nucleotide 1 through 1,059 (see, SEQ.ID.NO.:13) and amino acid residue 1 through 353 (see, SEQ.ID.NO.:14). With respect to the MCH receptor, 2 amino acid residues (an equivalent of 6 nucleotides) were placed in between the endogenous (or non-endogenous) GPCR and the start codon for the G protein $G_{i\alpha}$. Therefore, the Gi protein is located at nucleotide 1,066 through 2,133 (see, SEQ.ID.NO.:13) and at amino acid residue 356 through 711 (see, SEQ.ID.NO.:14). Those skilled in the art are credited with the ability to select techniques for constructing a GPCR Fusion Protein where the G protein is fused to the 3' end of the GPCR of interest.

Example 3583

ASSAY FOR DETERMINATION OF CONSTITUTIVE ACTIVITY OF NON-ENDOGENOUS GPCRS

A. Intracellular IP_3 Accumulation Assay

On day 1, cells comprising the receptors (endogenous and/or non-endogenous) can be plated onto 24 well plates, usually 1×10^5 cells/well (although this number can be optimized). On day 2 cells can be transfected by firstly mixing 0.25 μ g DNA in 50 μ l serum free DMEM/well and 2 μ l lipofectamine in 50 μ l serum-free DMEM/well. The solutions are gently mixed and incubated for 15-30 min at room temperature. Cells are washed with 0.5 ml PBS and 400 μ l of serum free media is mixed with the transfection media and added to the cells. The cells are then incubated for 3-4 hrs at $37^\circ\text{C}/5\%\text{CO}_2$ and then the transfection media is removed and replaced with 1ml/well of regular growth media. On day 3 the cells are labeled with ^3H -myo-inositol. Briefly, the media is removed and the cells are washed with 0.5 ml PBS. Then 0.5 ml inositol-free/serum free media (GIBCO BRL) is added/well with 0.25 μCi of ^3H -myo-inositol/ well and the cells are incubated for 16-18 hrs o/n at $37^\circ\text{C}/5\%\text{CO}_2$. On Day 4 the cells are washed with 0.5 ml PBS and 0.45 ml of assay medium is added containing inositol-free/serum free media 10 μM pargyline 10 mM lithium chloride or 0.4 ml of assay medium and 50 μ l of 10x

ketanserin (ket) to final concentration of 10 μ M. The cells are then incubated for 30 min at 37°C. The cells are then washed with 0.5 ml PBS and 200 μ l of fresh/ice cold stop solution (1M KOH; 18 mM Na-borate; 3.8 mM EDTA) is added/well. The solution is kept on ice for 5-10 min or until cells were lysed and then neutralized by 200 μ l of fresh/ice cold neutralization sol. (7.5 % HCL). The lysate is then transferred into 1.5 ml eppendorf tubes and 1 ml of chloroform/methanol (1:2) is added/tube. The solution is vortexed for 15 sec and the upper phase is applied to a Biorad AG1-X8™ anion exchange resin (100-200 mesh). Firstly, the resin is washed with water at 1:1.25 W/V and 0.9 ml of upper phase is loaded onto the column. The column is washed with 10 mls of 5 mM myo-inositol and 10 ml of 5 mM Na-borate/60mM Na-formate. The inositol tris phosphates are eluted into scintillation vials containing 10 ml of scintillation cocktail with 2 ml of 0.1 M formic acid/ 1 M ammonium formate. The columns are regenerated by washing with 10 ml of 0.1 M formic acid/3M ammonium formate and rinsed twice with H₂O and stored at 4°C in water.

Reference is made to Figure 1. Figure 1 provides an illustration of IP₃ production from several non-endogenous, constitutively activated version of MCH receptor as compared with the endogenous version of this receptor. When compared to the endogenous version of MCH receptor ("MCH-R wt"), MCH-IC3-SST2 evidenced about a 27% increase in IP₃ accumulation.

Example 3584

Determination of Compound Using [³⁵S]GTP γ S ASSAY

Direct identification of candidate compounds was initially screened using [³⁵S]GTP γ S Assay (see, Example 6 of co-pending patent application 09/826,509). Preferably, an MCH receptor: Gi Fusion Protein was utilized, according to Example 6(2) of co-pending patent application 09/826,509. Several lead hits were identified utilizing [³⁵S]GTP γ S Assay.

Example 3585

High Throughput Functional Screening: FLIPR™

Subsequently, a functional based assay was used to confirm the lead hits, referred to as FLIPR™ (the Fluorometric Imaging Plate Reader) and FDSS6000™ (Functional

Drug Screening System). This assay utilized a non-endogenous version of the MCH receptor, which was created by swapping the third intracellular loop of the MCH receptor with that of the SST2 receptor (see Example 2(B)(2) of patent application serial number 09/826,509).

The FLIPR and FDSS assays are able to detect intracellular Ca^{2+} concentration in cells, which can be utilized to assess receptor activation and determine whether a candidate compound is an, for example, antagonist, inverse agonist or agonist to a Gq-coupled receptor. The concentration of free Ca^{2+} in the cytosol of any cell is extremely low, whereas its concentration in the extracellular fluid and endoplasmic reticulum (ER) is very high. Thus, there is a large gradient tending to drive Ca^{2+} into the cytosol across both the plasma membrane and ER. The FLIPRTM and FDSS6000TM systems (Molecular Devices Corporation, HAMAMATSU Photonics K.K.) are designed to perform functional cell-based assays, such as the measurement of intracellular calcium for high-throughput screening. The measurement of fluorescent is associated with calcium release upon activation of the Gq-coupled receptors. Gi or Go coupled receptors are not as easily monitored through the FLIPRTM and FDSS6000TM systems because these G proteins do not couple with calcium signal pathways.

To confirm the lead hits identified using the [³⁵S]GTPγS assay, Fluorometric Imaging Plate Reader system was used to allow for rapid, kinetic measurements of intracellular fluorescence in 96 well microplates (or 384 well microplates). Simultaneous measurements of fluorescence in all wells can be made by FLIPR or FDSS6000TM every second with high sensitivity and precision. These systems are ideal for measuring cell-based functional assays such as monitoring the intracellular calcium fluxes that occur within seconds after activation of the Gq coupled receptor.

Briefly, the cells are seeded into 96 well at 5.5×10^4 cells/well with complete culture media (Dulbecco's Modified Eagle Medium with 10 % fetal bovine serum, 2 mM L-glutamine, 1 mM sodium pyruvate and 0.5 mg/ml G418, pH 7.4) for the assay next day. On the day of assay, the media is removed and the cells are incubated with 100 μl of loading buffer (4 μM Fluo4-AM in complete culture media containing 2.5 mM Probenicid, 0.5 mg/ml and 0.2% bovine serum albumin) in 5% CO₂ incubator at 37°C for 1 hr. The loading buffer is removed, and the cells are washed with wash buffer (Hank's Balanced Salt Solution containing 2.5 mM Probenicid, 20 mM HEPES, 0.5 mg/ml and 0.2% bovine

serum albumin, pH 7.4)). One hundred fifty μ l of wash buffer containing various concentrations of test compound are added to the cells, and the cells are incubated in 5% CO₂ incubator at 37°C for 30 min. Fifty μ l of wash buffer containing various concentration of MCH are added to each well, and transient changes in [Ca²⁺]_i evoked by MCH are monitored using the FLIPR or FDSS in 96 well plates at Ex. 488 nm and Em. 530 nm for 290 second. When antagonist activity of compound is tested, 50 nM of MCH is used.

Use of FLIPRTM and FDSS6000TM can be accomplished by following manufacturer's instruction (Molecular Device Corporation and HAMAMATSU Photonics K.K.).

The results were shpwn below.

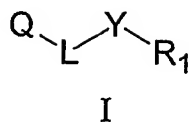
Compound No.	IC ₅₀ value (nM)
Example 41	6
Example 42	19

It is intended that each of the patents, applications, printed publications, and other published documents mentioned or referred to in this specification be herein incorporated by reference in their entirety.

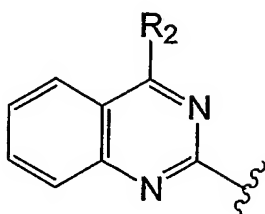
Those skilled in the art will appreciate that numerous changes and modifications may be made to the preferred embodiments of the invention and that such changes and modifications may be made without departing from the spirit of the invention. It is therefore intended that the appended claims cover all such equivalent variations as fall within the true spirit and scope of the invention.

What is claimed is:

1. A compound of Formula I:

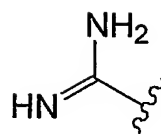


wherein Q is



II

or



III

R₁ represents

(i) C₁-C₁₆ alkyl,

C₁-C₁₆ alkyl substituted by substituent(s) independently selected from

•halogen,

•hydroxy,

•oxo,

•C₁-C₃ alkoxy,

•C₁-C₃ alkoxy substituted by substituent(s) independently selected from

••carbocyclic aryl,

••heterocyclyl,

••heterocyclyl substituted by C₁-C₃ alkyl,

•C₁-C₃ alkylcarbonyloxy,

•carbocyclyloxy,

•carbocyclic aryloxy,

•carbocyclic aryloxy substituted by substituent(s) independently selected from

••halogen,

••nitro,

••carbocyclic aryl,

••carbocyclic aryl substituted by C₁-C₃ alkoxy,

- C₁-C₄ alkyl,
- C₁-C₄ alkyl substituted by substituent(s) independently selected from
- oxo,
- mono- or di-C₁-C₃ alkylamino,
- mono- or di-C₁-C₃ alkylamino substituted by carbocyclic aryl,
- mono- or di-C₁-C₃ alkylamino substituted by halogenated carbocyclic aryl,
- carbocyclic arylcarbonylamino,
- halogenated carbocyclic arylcarbonylamino,
- heterocycloxy,
- heterocycloxy substituted by C₁-C₃ alkyl,
- substituted heterocycl-ethylideneaminooxy,
- C₁-C₃ alkoxy carbonyl,
- C₁-C₃ alkoxy carbonyl substituted by carbocyclic aryl,
- mono- or di-C₁-C₃ alkylaminocarbonyl,
- mono- or di-C₁-C₃ alkylamino,
- mono- or di-C₁-C₃ alkylamino substituted by substituent(s) independently selected from
- cyano,
- carbocyclic aryl,
- heterocyclyl,
- mono- or di-carbocyclic arylamino,
- mono- or di-carbocyclic arylamino substituted by substituent(s) independently selected from
- hydroxy,
- C₁-C₃ alkyl,
- C₁-C₃ alkylcarbonylamino,
- C₁-C₃ alkylcarbonylamino substituted by substituent(s) independently selected from
- C₁-C₃ alkylcarbonylamino,
- carbocyclic arylcarbonylamino,
- heterocyclyl,
- C₁-C₄ alkoxy carbonylamino,
- heterocycl carbonylamino,
- carbocyclic arylsulfonylamino,

- carbocyclic arylsulfonylamino substituted by substituent(s) independently selected from
 - nitro,
 - C₁-C₃ alkyl,
 - mono- or di-C₁-C₃ alkylamino,
- C₁-C₃ alkylthio,
- C₁-C₃ alkylthio substituted by substituent(s) independently selected from
 - mono- or di-carbocyclic arylaminocarbonyl,
 - halogenated mono- or di-carbocyclic arylaminocarbonyl,
 - mono- or di-carbocyclic arylamino,
 - halogenated mono- or di-carbocyclic arylamino,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkoxy,
 - carbocyclic arylthio,
 - carbocyclic arylthio substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - carbocyclic arylsulfonyl,
 - halogenated carbocyclic arylsulfonyl,
 - heterocyclylthio,
 - heterocyclylthio substituted by substituent(s) independently selected from
 - nitro,
 - C₁-C₃ alkyl,
 - C₃-C₆ cycloalkyl,
 - C₃-C₆ cycloalkyl substituted by C₁-C₃ alkyl,
 - C₃-C₆ cycloalkenyl,
 - carbocyclyl,
 - carbocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,

- C₂-C₃ alkenyl,
- C₂-C₃ alkenyl substituted by carbocyclic aryl,
- C₂-C₃ alkenyl substituted by carbocyclic aryl substituted C₁-C₃ alkylsulfinyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - oxo,
 - carbocyclic aryl,
 - heterocyclyl,
 - mono- or di-carbocyclic arylamino,
 - mono- or di-carbocyclic arylamino substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
 - halogenated C₁-C₃ alkoxy,
 - C₁-C₄ alkoxy,
 - C₁-C₄ alkoxy substituted by substituent(s) independently selected from
 - halogen,
 - carbocyclic aryl,
 - carbocyclic aryloxy,
 - C₁-C₃ alkoxycarbonyl,
 - C₁-C₃ alkylcarbonyloxy,
 - mono- or di-C₁-C₃ alkylamino,
 - mono- or di-carbocyclic arylamino,

- halogenated mono- or di-carbocyclic arylamino,
- mono- or di-carbocyclic arylaminocarbonyl,
- mono- or di-carbocyclic arylaminocarbonyl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
 - halogenated C₁-C₃ alkoxy,
 - mercapto,
 - C₁-C₃ alkylthio,
 - halogenated C₁-C₃ alkylthio,
 - C₁-C₃ alkylsulfonyl,
 - C₃-C₆ cycloalkyl,
 - carbocyclic aryl,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - hydroxy,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkyl substituted by carbocyclic aryl,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy substituted by carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
- (ii) C₂-C₈ alkenyl,
C₂-C₈ alkenyl substituted by substituent(s) independently selected from
 - halogen,
 - oxo,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy substituted by carbocyclic aryl,
 - carbocyclic aryl,

•carbocyclic aryl substituted by substituent(s) independently selected from

••halogen,

••hydroxy,

••nitro,

••C₁-C₃ alkyl,

••halogenated C₁-C₃ alkyl,

••C₁-C₃ alkoxy,

••halogenated C₁-C₃ alkoxy,

•heterocyclyl,

•heterocyclyl substituted by substituent(s) independently selected from

••hydroxy,

••nitro,

••C₁-C₃ alkyl,

••C₁-C₃ alkoxy,

(iii) C₂-C₄ alkynyl,

C₂-C₄ alkynyl substituted by carbocyclic aryl,

(iv) C₃-C₆ cycloalkyl,

C₃-C₆ cycloalkyl substituted by substituent(s) independently selected from

•C₁-C₃ alkyl,

•C₁-C₃ alkyl substituted by substituent(s) independently selected from

••hydroxy,

••oxo,

••carbocyclic aryl,

•mono- or di-C₁-C₃ alkylamino,

•mono- or di-C₁-C₃ alkylamino substituted by carbocyclic aryl,

•carbocyclic arylcarbonylamino,

•carbocyclic aryl,

(v) C₃-C₆ cycloalkyl,

C₃-C₆ cycloalkyl substituted by C₁-C₃ alkyl,

(vi) carbocyclyl,

carbocyclyl substituted by substituent(s) independently selected from

•hydroxy,

- nitro,
- (vii) carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - nitro,
 - C₁-C₉ alkyl,
 - C₁-C₉ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - oxo,
 - C₁-C₃ alkoxy,
 - carbocyclic aryloxy,
 - mono- or di-C₁-C₃ alkylamino-N-oxy,
 - mono- or di-C₁-C₃ alkylamino,
 - mono- or di-C₁-C₃ alkylamino substituted by carbocyclic aryl,
 - mono- or di-carbocyclic arylamino,
 - carbocyclylimino,
 - carbocyclylimino substituted by carbocyclic aryl,
 - mono- or di-carbocyclic arylamino,
 - mono- or di-carbocyclic arylamino substituted by C₁-C₃ alkoxy,
 - mono- or di-carbocyclic arylaminocarbonyl,
 - mono- or di-carbocyclic arylaminocarbonyl substituted by C₁-C₃ alkoxy,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl,
 - heterocyclyl,
 - heterocyclyl substituted by C₁-C₃ alkyl,
 - C₂-C₃ alkenyl,

- C₂-C₃ alkenyl substituted by carbocyclic aryl,
- C₁-C₉ alkoxy,
- C₁-C₉ alkoxy substituted by substituent(s) independently selected from
 - hydroxy,
 - halogen,
 - carboxy,
 - mono- or di-C₁-C₃ alkylamino,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl,
- C₂-C₃ alkenyloxy,
- C₁-C₃ alkylcarbonyloxy,
- carbocyclic aryloxy,
- carbocyclic aryloxy substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₄ alkyl,
 - halogenated C₁-C₄ alkyl,
 - C₁-C₃ alkoxy,
 - heterocyclyloxy,
 - heterocyclyloxy substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl,
- (carbocyclic aryl)S(O)₂O,

- carboxy,
- C₁-C₃ alkoxycarbonyl,
- mono- or di-C₁-C₃ alkylaminocarbonyl,
- mono- or di-C₁-C₃ alkylaminocarbonyl substituted by carbocyclic aryl,
- mono- or di-carbocyclic arylaminocarbonyl,
- mono- or di-carbocyclic arylaminocarbonyl substituted by C₁-C₃ alkyl,
- amino,
- mono- or di-C₁-C₄ alkylamino,
- mono- or di-C₁-C₄ alkylamino substituted by cyano,
- mono- or di-carbocyclic arylamino,
- C₁-C₃ alkynylcarbonylamino,
- C₁-C₃ alkynylcarbonylamino substituted by carbocyclic aryl,
- carbocyclic arylsulfonylamino,
- carbocyclic arylsulfonylamino substituted by C₁-C₃ alkyl,
- (carbocyclic aryl)NHC(O)NH,
- (carbocyclic aryl)NHC(O)NH substituted by C₁-C₃ alkoxy,
- (carbocyclic aryl)NHC(O)NH substituted by halogenated C₁-C₃ alkoxy,
- carbocyclic aryl diazo,
- carbocyclic aryl diazo substituted by mono- or di- C₁-C₃ alkylamino,
- C₁-C₃ alkylthio,
- halogenated C₁-C₃ alkylthio,
- carbocyclic arylthio,
- carbocyclic arylthio substituted by substituent(s) independently selected from
 - halogen,
 - cyano,
 - C₁-C₃ alkyl,
 - heterocyclylthio,
 - C₁-C₃ alkylsulfonyl,
 - mono- or di-C₁-C₃ alkylaminosulfonyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - C₁-C₇ alkyl,

- halogenated C₁-C₇ alkyl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
 - C₁-C₃ alkyl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
- (viii) heterocyclyl,
or heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - oxo,
 - C₁-C₃ alkylcarbonyloxy,
 - carbocyclic arylcarbonylamino,
 - halogenated carbocyclic arylcarbonylamino,
 - C₁-C₃ alkoxycarbonyl,
 - C₁-C₃ alkylthio,
 - C₁-C₃ alkylthio substituted by carbocyclic aryl,
 - C₁-C₃ alkylthio substituted by halogenated carbocyclic aryl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,

- halogenated C₁-C₃ alkyl,
- C₁-C₃ alkoxy,
- C₁-C₃ alkoxy substituted by carbocyclic aryl,
- carbocyclic aryloxy,
- carbocyclic aryloxy substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - mono- or di-C₁-C₃ alkylamino,
 - C₁-C₄ alkylcarbonylamino,
 - C₁-C₃ alkylthio,
 - C₁-C₃ alkenylthio,
 - carbocyclic arylthio,
 - halogenated carbocyclic arylthio,
 - carbocyclic arylthio substituted by C₁-C₃ alkoxycarbonyl,
 - heterocyclylthio,
 - heterocyclylthio substituted by C₁-C₃ alkyl,
 - C₁-C₃ alkylsulfonyl,
 - carbocyclic arylsulfonyl,
 - halogenated carbocyclic arylsulfonyl,
 - carbocyclic arylsulfonyl substituted by C₁-C₄ alkyl,
 - C₁-C₃ alkoxycarbonyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
 - halogenated C₁-C₃ alkoxy,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - halogen,

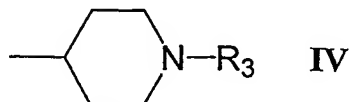
- C₁-C₃ alkyl,
- halogenated C₁-C₃ alkyl,
- C₁-C₃ alkoxy,
- C₁-C₃ alkoxycarbonyl;

R₂ is -NHNH₂, -NHNHBoc, -N(R_{2a})(R_{2b}), morpholino, 4-acetyl-piperazyl, or 4-phenyl-piperazyl;

wherein R_{2a} is H or C₁-C₃ alkyl;

R_{2b} is C₁-C₄ alkyl, C₁-C₄ alkyl substituted by substituent(s) independently selected from

- hydroxy,
 - C₁-C₃ alkoxy,
 - amino,
 - NHBoc,
 - C₃-C₆ cycloalkyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
 - SO₂NH₂,
 - heterocyclyl,
 - C₃-C₆ cycloalkyl, carbocyclic aryl, carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
- or a group of Formula IV;

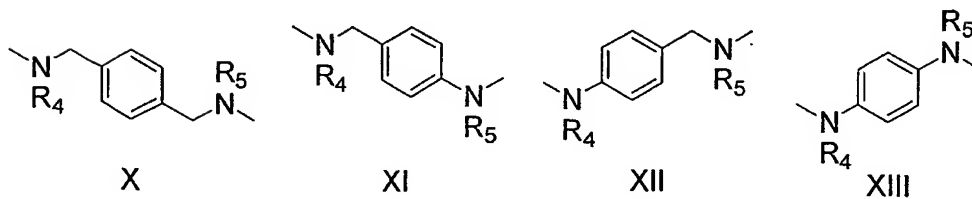
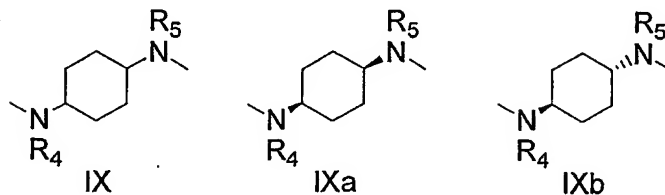
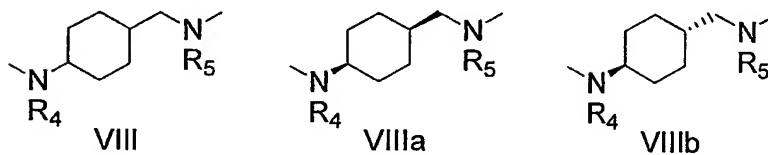
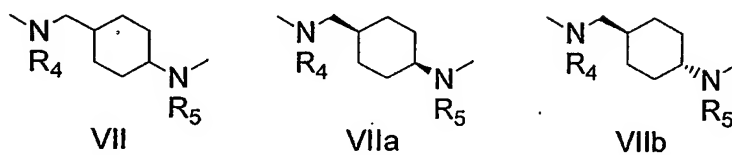
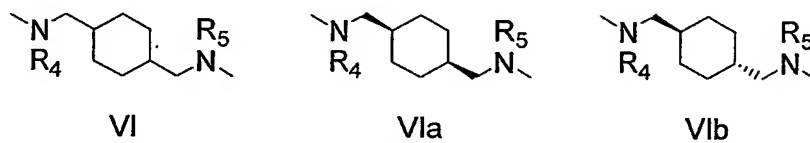
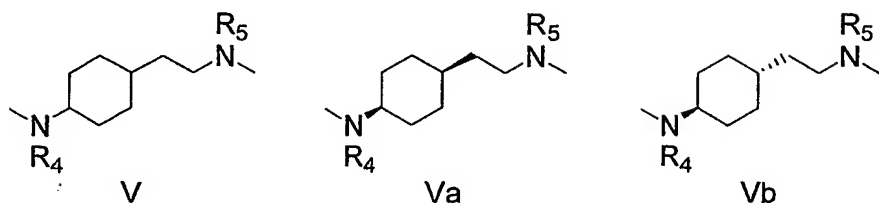


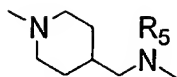
wherein Boc is carbamic acid *tert*-butyl ester and R₃ is C₁-C₃ alkyl or C₁-C₃ alkyl

substituted by substituent(s) independently selected from

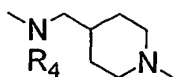
- carbocyclic aryl,
- halogenated carbocyclic aryl,
- carbocyclic aryl substituted by C₁-C₃ alkoxy;

L is selected from Formula V - XIX;

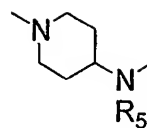




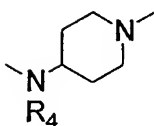
XIV



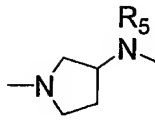
XV



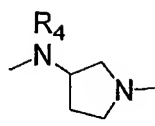
XVI



XVII



XVIII



XIX

wherein R_4 is H or C_1 - C_3 alkyl;

R_5 is H, C_1 - C_3 alkyl, or C_1 - C_3 alkyl substituted by a substituted carbocyclic aryl;

Y is $-S(O)_2-$, $-C(O)-$, or $-(CH_2)_m$;

m is 0 or 1;

wherein carbocyclic aryl is phenyl, naphthyl, anthranyl, biphenyl, or phenanthryl;

carbocyclyl is 10,11-dihydro-5-oxo-dibenzo[a,d]cycloheptyl, 1-oxo-indanyl, 7,7-dimethyl-2-oxo-bicyclo[2.2.1]heptyl, 9H-fluorenyl, 9-oxo-fluorenyl, acenaphthyl, anthraquinonyl, C-fluoren-9-ylidene, indanyl, indenyl, 1,2,3,4-tetrahydro-naphthyl, or bicyclo[2.2.1]hepteny;

heterocyclyl is 1,2,3,4-tetrahydro-isoquinolyl, 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1,3,4-thiadiazolyl, 1,3-dioxo-isoindolyl, 1,3-dioxolanyl, 1H-indolyl, 1H-pyrrolo[2,3-c]pyridyl, 1H-pyrrolyl, 1-oxo-3H-isobenzofuranyl, 2,2',5',2"-terthiophenyl, 2,2'-bithiophenyl, 2,3-dihydro-1-oxo-isoindolyl, 2,3-dihydro-benzo[1,4]dioxinyl, 2,4-dihydro-3-oxo-pyrazolyl, 2H-benzopyranyl, 2-oxo-benzopyranyl, 2-oxo-pyrrolidinyl, 3,4-dihydro-2H-benzo[1,4]oxazinyl, 3,4-dihydro-2H-benzo[b][1,4]dioxepinyl, 4H-benzo[1,3]dioxinyl, 4H-benzopyranyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, 4-oxo-3,4-dihydro-phthalazinyl, 4-oxo-benzopyranyl, 9,10,10-trioxo-thioxanthenyl, 9H-carbazolyl, 9H-xanthenyl, azetidiny, benzimidazolyl, benzo[1,3]dioxolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, benzofuryl, benzothiazolyl, cinnolyl, furyl, imidazo[2,1-b]thiazolyl, imidazolyl, isoxazolyl, morpholino, morpholinyl, oxazolyl, oxolanyl, piperazyl, piperidyl, piridyl, pyrazolo[5,1-b]thiazolyl, pyrazolyl, pyridyl, pyrimidyl, pyrrolidyl, quinolyl, quinoxalyl, thiazolidyl, thiazolyl, thienyl, thiolanyl, 2,3-

dihydro-benzofuryl, tetrahydro-thienyl, or benzofuranyl;
 halogen is fluoro, chloro, bromo, or iodo;
 or a salt thereof.

2. A compound according to claim 1, wherein Q is Formula II;
 R₁ represents

- (i) C₁-C₁₀ alkyl,
- C₁-C₁₀ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - oxo,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy substituted by carbocyclic aryl,
 - C₁-C₃ alkylcarbonyloxy,
 - carbocycloxy,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - oxo,
 - carbocyclic arylcarbonylamino,
 - halogenated carbocyclic arylcarbonylamino,
 - heterocycloxy,
 - heterocycloxy substituted by C₁-C₃ alkyl,
 - substituted heterocyclyl-ethylideneaminoxy,
 - C₁-C₃ alkoxycarbonyl,
 - C₁-C₃ alkoxycarbonyl substituted by carbocyclic aryl,
 - mono- or di-C₁-C₃ alkylaminocarbonyl,
 - mono- or di-carbocyclic arylamino,
 - mono- or di-carbocyclic arylamino substituted by hydroxy,
 - C₁-C₃ alkylcarbonylamino,

- C₁-C₃ alkylcarbonylamino substituted by substituent(s) independently selected from
 - C₁-C₃ alkylcarbonylamino,
 - carbocyclic arylcarbonylamino,
 - heterocyclyl,
- C₁-C₄ alkoxy carbonylamino,
- heterocyclyl carbonylamino,
- carbocyclic arylsulfonylamino,
- carbocyclic arylsulfonylamino substituted by substituent(s) independently selected from
 - nitro,
 - C₁-C₃ alkyl,
 - mono- or di-C₁-C₃ alkylamino,
 - C₁-C₃ alkylthio,
 - C₁-C₃ alkylthio substituted by substituent(s) independently selected from
 - mono- or di-carbocyclic arylaminocarbonyl,
 - halogenated mono- or di-carbocyclic arylaminocarbonyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkoxy,
 - carbocyclic arylthio,
 - carbocyclic arylthio substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - carbocyclic arylsulfonyl,
 - halogenated carbocyclic arylsulfonyl,
 - heterocyclylthio,
 - heterocyclylthio substituted by substituent(s) independently selected from
 - nitro,
 - C₁-C₃ alkyl,
 - C₃-C₆ cycloalkyl,
 - C₃-C₆ cycloalkyl substituted by C₁-C₃ alkyl,
 - C₃-C₆ cycloalkenyl,

- carbocyclyl,
- carbocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
 - C₂-C₃ alkenyl,
 - C₂-C₃ alkenyl substituted by carbocyclic aryl,
 - C₂-C₃ alkenyl substituted by carbocyclic aryl substituted C₁-C₃ alkylsulfinyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - oxo,
 - carbocyclic aryl,
 - heterocyclyl,
 - C₁-C₄ alkoxy,
 - C₁-C₄ alkoxy substituted by substituent(s) independently selected from
 - halogen,
 - carbocyclic aryl,
 - carbocyclic aryloxy,
 - C₁-C₃ alkylcarbonyloxy,
 - mono- or di-carbocyclic arylamino,
 - halogenated mono- or di-carbocyclic arylamino,
 - mono- or di-carbocyclic arylaminocarbonyl,
 - mono- or di-carbocyclic arylaminocarbonyl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₃ alkyl,

- C₁-C₃ alkoxy,
- halogenated C₁-C₃ alkoxy,
- mercapto,
- C₁-C₃ alkylthio,
- halogenated C₁-C₃ alkylthio,
- C₁-C₃ alkylsulfonyl,
- C₃-C₆ cycloalkyl,
- carbocyclic aryl,
- heterocyclyl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
- hydroxy,
- C₁-C₃ alkyl,
- C₁-C₃ alkyl substituted by carbocyclic aryl,
- C₁-C₃ alkoxy,
- C₁-C₃ alkoxy substituted by carbocyclic aryl,
- carbocyclic aryl,
- halogenated carbocyclic aryl,
- (ii) C₂-C₆ alkenyl,
- C₂-C₆ alkenyl substituted by substituent(s) independently selected from
- oxo,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
- halogen,
- nitro,
- C₁-C₃ alkyl,
- halogenated C₁-C₃ alkyl,
- C₁-C₃ alkoxy,
- halogenated C₁-C₃ alkoxy,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
- hydroxy,

- C₁-C₃ alkyl,
- C₁-C₃ alkoxy,
- (iii) C₃-C₆ cycloalkyl,
C₃-C₆ cycloalkyl substituted by substituent(s) independently selected from
 - C₁-C₃ alkyl,
 - C₁-C₃ alkyl substituted by substituent(s) independently selected from
 - oxo,
 - carbocyclic aryl,
 - carbocyclic arylcarbonylamino,
 - carbocyclic aryl,
 - (iv) carbocyclyl,
carbocyclyl substituted by nitro,
 - (v) carbocyclic aryl,
carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - nitro,
 - C₁-C₉ alkyl,
 - C₁-C₉ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - oxo,
 - carbocyclic aryloxy,
 - carbocyclylimino,
 - carbocyclylimino substituted by carbocyclic aryl,
 - mono- or di-carbocyclic arylaminocarbonyl,
 - mono- or di-carbocyclic arylaminocarbonyl substituted by C₁-C₃ alkoxy,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl,

- heterocyclyl,
- heterocyclyl substituted by C₁-C₃ alkyl,
- C₁-C₇ alkoxy,
- C₁-C₇ alkoxy substituted by substituent(s) independently selected from
 - halogen,
 - carbocyclic aryl,
 - C₁-C₃ alkylcarbonyloxy,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by C₁-C₃ alkoxy,
 - C₁-C₃ alkoxycarbonyl,
 - mono- or di-C₁-C₃ alkylaminocarbonyl,
 - mono- or di-C₁-C₃ alkylaminocarbonyl substituted by carbocyclic aryl,
 - mono- or di-carbocyclic arylaminocarbonyl,
 - mono- or di-carbocyclic arylaminocarbonyl substituted by C₁-C₃ alkyl,
 - amino,
 - mono- or di-C₁-C₃ alkylamino,
 - C₁-C₃ alkynylcarbonylamino,
 - C₁-C₃ alkynylcarbonylamino substituted by carbocyclic aryl,
 - carbocyclic arylsulfonylamino,
 - carbocyclic arylsulfonylamino substituted by C₁-C₃ alkyl,
 - (carbocyclic aryl)NHC(O)NH,
 - (carbocyclic aryl)NHC(O)NH substituted by C₁-C₃ alkoxy,
 - (carbocyclic aryl)NHC(O)NH substituted by halogenated C₁-C₃ alkoxy,
 - C₁-C₃ alkylthio,
 - halogenated C₁-C₃ alkylthio,
 - carbocyclic arylthio,
 - carbocyclic arylthio substituted by cyano,
 - C₁-C₃ alkylsulfonyl,
 - mono- or di-C₁-C₃ alkylaminosulfonyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - C₁-C₇ alkyl,

- halogenated C₁-C₇ alkyl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
 - C₁-C₃ alkyl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
- (vi) heterocyclyl,
- or heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - oxo,
 - C₁-C₃ alkylthio,
 - C₁-C₃ alkylthio substituted by carbocyclic aryl,
 - C₁-C₃ alkylthio substituted by halogenated carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - heterocyclyl,
 - C₁-C₃ alkoxy,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkylthio,
 - C₁-C₃ alkenylthio,
 - carbocyclic arylthio,
 - C₁-C₃ alkylsulfonyl,
 - carbocyclic arylsulfonyl,
 - halogenated carbocyclic arylsulfonyl,
 - carbocyclic arylsulfonyl substituted by C₁-C₄ alkyl,

- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl;

Y is -C(O)-;

wherein carbocyclic aryl is phenyl, naphthyl, anthranyl, or biphenyl;

carbocyclyl is 10,11-dihydro-5-oxo-dibenzo[a,d]cycloheptyl, 1-oxo-indanyl, 9H-fluorenyl, 9-oxo-fluorenyl, acenaphthyl, anthraquinonyl, C-fluoren-9-ylidene, indanyl, indenyl, 1,2,3,4-tetrahydro-naphthyl, or bicyclo[2.2.1]hepteny;

heterocyclyl is 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1,3-dioxo-isindolyl, 1H-indolyl, 1H-pyrrolyl, 1-oxo-3H-isobenzofuranyl, 2,3-dihydro-benzo[1,4]dioxinyl, 2,3-dihydro-benzofuryl, 2,4-dihydro-3-oxo-pyrazolyl, 2H-benzopyranyl, 2-oxo-benzopyranyl, 2-oxo-pyrrolidinyl, 3,4-dihydro-2H-benzo[b][1,4]dioxepinyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, 4-oxo-3,4-dihydro-phthalazinyl, 4-oxo-benzopyranyl, 9,10,10-trioxo-thioxanthenyl, 9H-xanthenyl, azetidiny, benzimidazolyl, benzo[1,3]dioxolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, cinnolyl, furyl, imidazolyl, isoxazolyl, morpholino, morpholinyl, oxazolyl, oxolanyl, piperidyl, piridyl, pyrazolyl, pyridyl, pyrimidyl, pyrrolidyl, quinolyl, quinoxalyl, thiazolidyl, thiazolyl, thienyl, thiolanyl, tetrahydro-thienyl, benzofuranyl, or benzothiazolyl;

halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

3. A compound according to claim 2, wherein

R₁ represents

(i) C₁-C₁₀ alkyl,

C₁-C₁₀ alkyl substituted by substituent(s) independently selected from

- oxo,
- di-propylaminocarbonyl,
- methoxy substituted by carbocyclic aryl,
- methylcarbonyloxy,
- carbocyclic aryloxy,
- halogenated carbocyclic aryloxy,
- carbocyclic aryloxy substituted by nitro,
- heterocyclyloxy substituted by methyl,
- substituted heterocyclyl-ethylideneaminoxy,
- tert*-butoxycarbonylamino,
- carbocyclic arylcarbonylamino,
- C₁-C₂ alkylthio,
- C₁-C₂ alkylthio substituted by substituent(s) independently selected from
 - halogenated carbocyclic aryl,
 - carbocyclic aryl substituted by methoxy,
 - carbocyclic arylthio,
 - heterocyclylthio substituted by nitro,
 - heterocyclylthio substituted by methyl,
 - C₅-C₆ cycloalkyl,
 - C₅-C₆ cycloalkenyl,
 - carbocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - methyl,
 - methoxy,
 - ethenyl substituted by carbocyclic aryl substituted methylsulfinyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from

- oxo,
- carbocyclic aryl,
- heterocyclyl,
- C₁-C₄ alkoxy,
- halogenated C₁-C₄ alkoxy,
- C₁-C₄ alkoxy substituted by carbocyclic aryl,
- carbocyclic aryloxy,
- halogenated mono-carbocyclic arylaminocarbonyl,
- carbocyclic aryl,
- heterocyclyl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
- C₁-C₂ alkyl,
- C₁-C₂ substituted by carbocyclic aryl,
- methoxy,
- methoxy substituted by carbocyclic aryl,
- carbocyclic aryl,
- halogenated carbocyclic aryl,
- (ii) C₂-C₃ alkenyl substituted by substituent(s) independently selected from
- carbocyclic aryl,
- halogenated carbocyclic aryl,
- carbocyclic aryl substituted by nitro,
- (iii) C₃-C₆ cycloalkyl,
- C₃-C₆ cycloalkyl substituted by substituent(s) independently selected from
- methyl substituted by oxo,
- methyl substituted by carbocyclic aryl,
- carbocyclic aryl,
- (iv) carbocyclyl,
- (v) carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
- halogen,
- hydroxy,

- cyano,
- nitro,
- C₁-C₉ alkyl,
- C₁-C₉ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - oxo,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by methyl,
 - carbocyclic aryloxy,
 - C₁-C₇ alkoxy,
 - halogenated C₁-C₇ alkoxy,
 - C₁-C₇ alkoxy substituted by carbocyclic aryl,
 - methylcarbonyloxy,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by methoxy,
- amino,
- di-methylamino,
- propargynylcarbonylamino substituted by carbocyclic aryl,
- carbocyclic arylsulfonylamino substituted by methyl,
- (carbocyclic aryl)NHC(O)NH substituted by halogenated methoxy,
- halogenated methylthio,
- carbocyclic arylthio substituted by cyano,
- di-propylamino sulfonyl,
- mono- or di- ethylaminocarbonyl substituted by carbocyclic aryl,
- carbocyclic aryl,
- heterocyclyl substituted by methyl,
- heterocyclyl substituted by halogenated carbocyclic aryl,
- (vi) heterocyclyl,
- or heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₄ alkyl,

- C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - methylthio substituted by halogenated carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - heterocyclyl,
 - methoxy,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by methyl,
 - C₁-C₃ alkylthio,
 - propenylthio,
 - carbocyclic arylthio,
 - C₁-C₃ alkylsulfonyl,
 - carbocyclic arylsulfonyl substituted by C₁-C₄ alkyl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - carbocyclic aryl substituted by methyl,
 - carbocyclic aryl substituted by nitro,
 - heterocyclyl;

R₂ is methylamino or dimethylamino;

L is selected from Formula Va, VIIIa, or IXa;

wherein R₄ and R₅ are independently selected from H or C₁-C₃ alkyl;

wherein carbocyclic aryl is phenyl, naphthyl, anthranyl, or biphenyl;

carbocyclyl is 1-oxo-indanyl, 9-oxo-fluorenyl, indenyl, anthraquinonyl, C-fluoren-9-ylidene, 1,2,3,4-tetrahydro-naphthyl, or bicyclo[2.2.1]hepteny;

heterocyclyl is 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1,3-dioxo-isindolyl, 1*H*-indolyl, 1*H*-pyrrolyl, 1-oxo-3*H*-isobenzofuranyl, 2,3-dihydro-benzo[1,4]dioxinyl, 2,4-dihydro-3-oxo-pyrazolyl, 2*H*-benzopyranyl, 2-oxo-benzopyranyl, 3,4-dihydro-2*H*-benzo[b][1,4]dioxepinyl, 4-oxo-3,4-dihydro-phthalazinyl, 4-oxo-benzopyranyl, 9,10,10-trioxo-thioxanthenyl, 9*H*-xanthenyl, azetidiny, benzimidazolyl, benzo[1,3]dioxolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, furyl, imidazolyl, isoxazolyl, morpholino, morpholinyl, oxolanyl, piperidyl, piridyl, pyrazolyl, pyridyl, quinolyl,

quinoxalyl, thiazolidyl, thiazolyl, thienyl, thiolanyl, 2,3-dihydro-1-oxo-isoindolyl, 2,3-dihydro-benzofuryl, 2-oxo-pyrrolidinyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, cinnolyl, pyrimidyl, pyrrolidyl, tetrahydro-thienyl, benzofuranyl, or benzothiazolyl;

halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

4. A compound according to claim 3, wherein

R₁ represents

(i) C₁-C₁₀ alkyl substituted by substituent(s) independently selected from

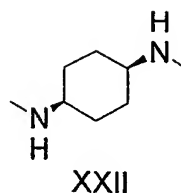
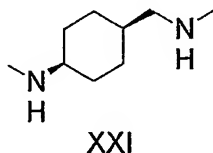
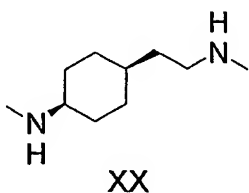
- oxo,
- di-propylaminocarbonyl,
- methoxy substituted by carbocyclic aryl,
- methylcarbonyloxy,
- carbocyclic aryloxy,
- halogenated carbocyclic aryloxy,
- carbocyclic aryloxy substituted by nitro,
- heterocyclyloxy substituted by methyl,
- substituted heterocyclyl-ethylideneaminoxy,
- tert*-butoxycarbonylamino,
- carbocyclic arylcarbonylamino,
- C₁-C₂ alkylthio,
- C₁-C₂ alkylthio substituted by substituent(s) independently selected from
 - halogenated carbocyclic aryl,
 - carbocyclic aryl substituted by methoxy,
 - carbocyclic arylthio,
 - heterocyclylthio substituted by nitro,
 - heterocyclylthio substituted by methyl,
- C₅-C₆ cycloalkenyl,
- carbocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - methyl,
 - methoxy,

- ethenyl substituted by carbocyclic aryl substituted methylsulfinyl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - oxo,
 - carbocyclic aryl,
 - heterocyclyl,
 - C₁-C₄ alkoxy,
 - halogenated C₁-C₄ alkoxy,
 - C₁-C₄ alkoxy substituted by carbocyclic aryl,
 - carbocyclic aryloxy,
 - halogenated mono-carbocyclic arylaminocarbonyl,
 - carbocyclic aryl,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - C₁-C₂ alkyl,
 - C₁-C₂ substituted by carbocyclic aryl,
 - methoxy,
 - methoxy substituted by carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
- (ii) C₂-C₃ alkenyl substituted by substituent(s) independently selected from
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - carbocyclic aryl substituted by nitro,
- (iii) C₃-C₆ cycloalkyl substituted by substituent(s) independently selected from
 - methyl substituted by oxo,
 - methyl substituted by carbocyclic aryl,
 - carbocyclic aryl,

- (iv) carbocyclyl,
- (v) carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - nitro,
 - C₁-C₉ alkyl,
 - C₁-C₉ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - oxo,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by methyl,
 - carbocyclic aryloxy,
 - C₁-C₇ alkoxy,
 - halogenated C₁-C₇ alkoxy,
 - C₁-C₇ alkoxy substituted by carbocyclic aryl,
 - methylcarbonyloxy,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by methoxy,
 - amino,
 - di-methylamino,
 - propargynylcarbonylamino substituted by carbocyclic aryl,
 - carbocyclic arylsulfonylamino substituted by methyl,
 - (carbocyclic aryl)NHC(O)NH substituted by halogenated methoxy,
 - halogenated methylthio,
 - carbocyclic arylthio substituted by cyano,
 - di-propylamino sulfonyl,
 - mono- or di- ethylaminocarbonyl substituted by carbocyclic aryl,
 - carbocyclic aryl,
 - heterocyclyl substituted by methyl,
 - heterocyclyl substituted by halogenated carbocyclic aryl,
- (vi) or heterocyclyl substituted by substituent(s) independently selected from

- halogen,
- nitro,
- C₁-C₄ alkyl,
- C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - methylthio substituted by halogenated carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - heterocyclyl,
 - methoxy,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by methyl,
 - C₁-C₃ alkylthio,
 - propenylthio,
 - carbocyclic arylthio,
 - C₁-C₃ alkylsulfonyl,
 - carbocyclic arylsulfonyl,
 - carbocyclic arylsulfonyl substituted by C₁-C₄ alkyl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - carbocyclic aryl substituted by methyl,
 - carbocyclic aryl substituted by nitro,
 - heterocyclyl;

L is selected from Formula XX - XXII;



wherein carbocyclic aryl is phenyl, naphthyl, or biphenyl;

carbocyclyl is 1-oxo-indanyl, 9-oxo-fluorenyl, indenyl, anthraquinonyl, C-fluoren-

9-ylidene, 1,2,3,4-tetrahydro-naphthyl, or bicyclo[2.2.1]heptenyl;

heterocyclyl is 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1*H*-indolyl, 1*H*-pyrrolyl, 2,4-dihydro-3-oxo-pyrazolyl, 2*H*-benzopyranyl, 4-oxo-benzopyranyl, azetidiny, benzo[b]thienyl, furyl, isoxazolyl, morpholinyl, piperidyl, piridyl, pyrazolyl, pyridyl, quinolyl, thiazolidyl, thiazolyl, thienyl, thiolanyl, 2,3-dihydro-1-oxo-isoindolyl, 2,3-dihydro-benzofuryl, 2-oxo-benzopyranyl, 2-oxo-pyrrolidinyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, 9*H*-xanthenyl, cinnolyl, imidazolyl, morpholino, pyrimidyl, pyrrolidyl, tetrahydro-thienyl, benzofuranyl, or benzothiazolyl;

halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

5. A compound according to claim 4, wherein

R₁ represents

(i) C₁-C₅ alkyl substituted by substituent(s) independently selected from

- oxo,
- di-propylaminocarbonyl,
- methoxy substituted by carbocyclic aryl,
- methylcarbonyloxy,
- carbocyclic aryloxy,
- halogenated carbocyclic aryloxy,
- carbocyclic aryloxy substituted by nitro,
- heterocyclyloxy substituted by methyl,
- substituted heterocyclyl-ethylideneaminoxy,
- tert*-butoxycarbonylamino,
- carbocyclic arylcarbonylamino,
- C₁-C₂ alkylthio,
- C₁-C₂ alkylthio substituted by substituent(s) independently selected from
- halogenated carbocyclic aryl,
- carbocyclic aryl substituted by methoxy,
- carbocyclic arylthio,
- heterocyclylthio substituted by nitro,
- heterocyclylthio substituted by methyl,

- cyclohexenyl,
- carbocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - methyl,
 - methoxy,
 - ethenyl substituted by carbocyclic aryl substituted methylsulfinyl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - oxo,
 - carbocyclic aryl,
 - heterocyclyl,
 - C₁-C₂ alkoxy,
 - halogenated C₁-C₂ alkoxy,
 - C₁-C₂ alkoxy substituted by carbocyclic aryl,
 - carbocyclic aryloxy,
 - halogenated mono-carbocyclic arylaminocarbonyl,
 - carbocyclic aryl,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - C₁-C₂ alkyl,
 - C₁-C₂ substituted by carbocyclic aryl,
 - methoxy,
 - methoxy substituted by carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
- (ii) C₂-C₃ alkenyl substituted by substituent(s) independently selected from
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,

- carbocyclic aryl substituted by nitro,
- (iii) C₃-C₆ cycloalkyl substituted by substituent(s) independently selected from
 - methyl substituted by oxo,
 - methyl substituted by carbocyclic aryl,
 - carbocyclic aryl,
- (iv) carbocyclyl,
- (v) carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₂ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - oxo,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by methyl,
 - carbocyclic aryloxy,
 - C₁-C₂ alkoxy,
 - halogenated C₁-C₂ alkoxy,
 - C₁-C₂ alkoxy substituted by carbocyclic aryl,
 - methylcarbonyloxy,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by methoxy,
 - amino,
 - di-methylamino,
 - propargynylcarbonylamino substituted by carbocyclic aryl,
 - carbocyclic arylsulfonylamino substituted by methyl,
 - (carbocyclic aryl)NHC(O)NH substituted by halogenated methoxy,
 - halogenated methylthio,
 - carbocyclic arylthio substituted by cyano,
 - di-propylamino sulfonyl,

- mono- or di- ethylaminocarbonyl substituted by carbocyclic aryl,
- carbocyclic aryl,
- heterocyclyl substituted by methyl,
- heterocyclyl substituted by halogenated carbocyclic aryl,
- (vi) or heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - methylthio substituted by halogenated carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - heterocyclyl,
 - methoxy,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by methyl,
 - C₁-C₃ alkylthio,
 - propenylthio,
 - carbocyclic arylthio,
 - C₁-C₃ alkylsulfonyl,
 - carbocyclic arylsulfonyl,
 - carbocyclic arylsulfonyl substituted by methyl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - carbocyclic aryl substituted by methyl,
 - carbocyclic aryl substituted by nitro,
 - heterocyclyl;

wherein carbocyclic aryl is phenyl, naphthyl, or biphenyl;

carbocyclyl is 1-oxo-indanyl, indenyl, 9-oxo-fluorenyl, 1,2,3,4-tetrahydro-naphthyl, or bicyclo[2.2.1]hepteny;

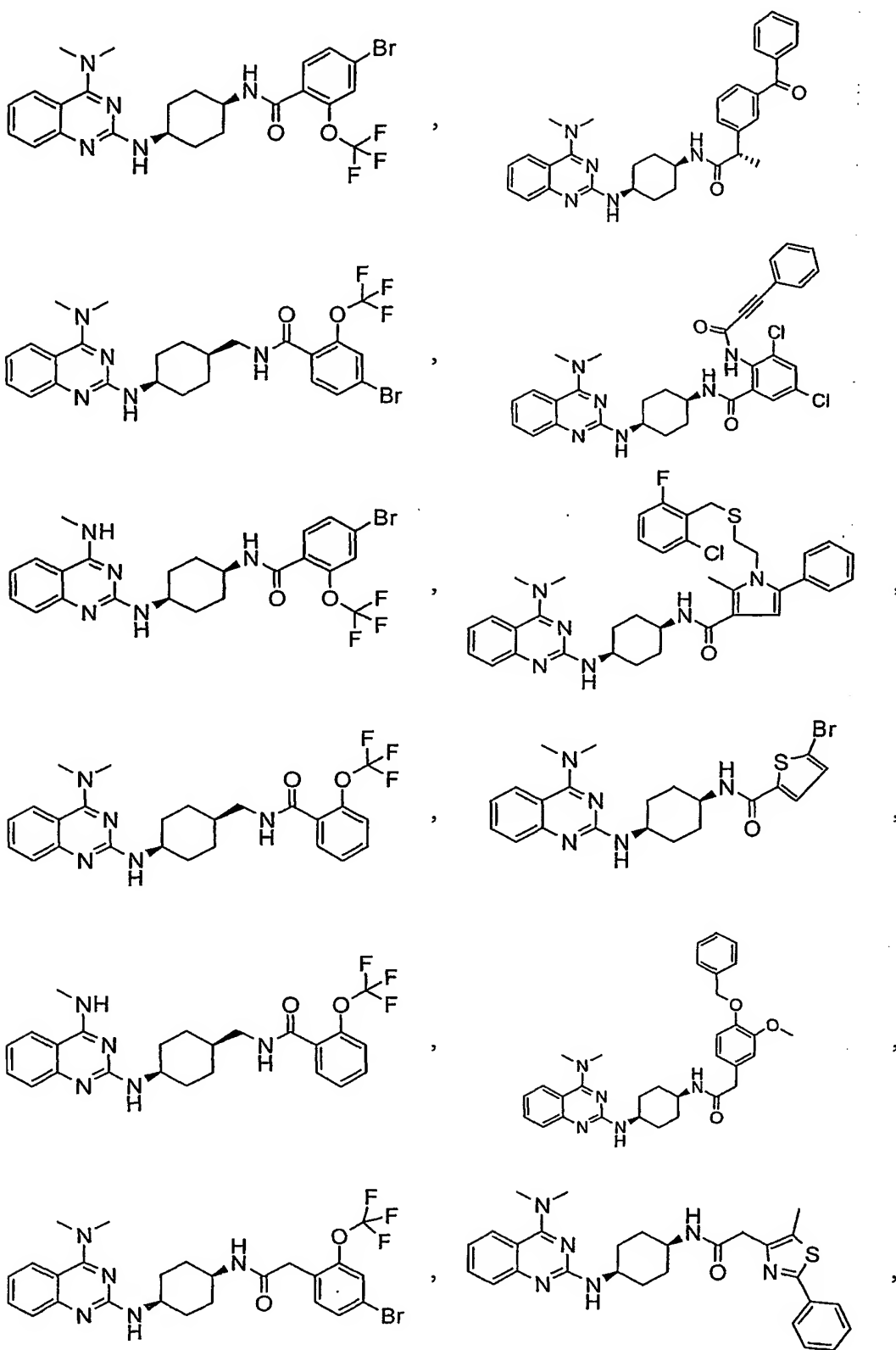
heterocyclyl is 1*H*-indolyl, 2,4-dihydro-3-oxo-pyrazolyl, furyl, pyrazolyl, pyridyl,

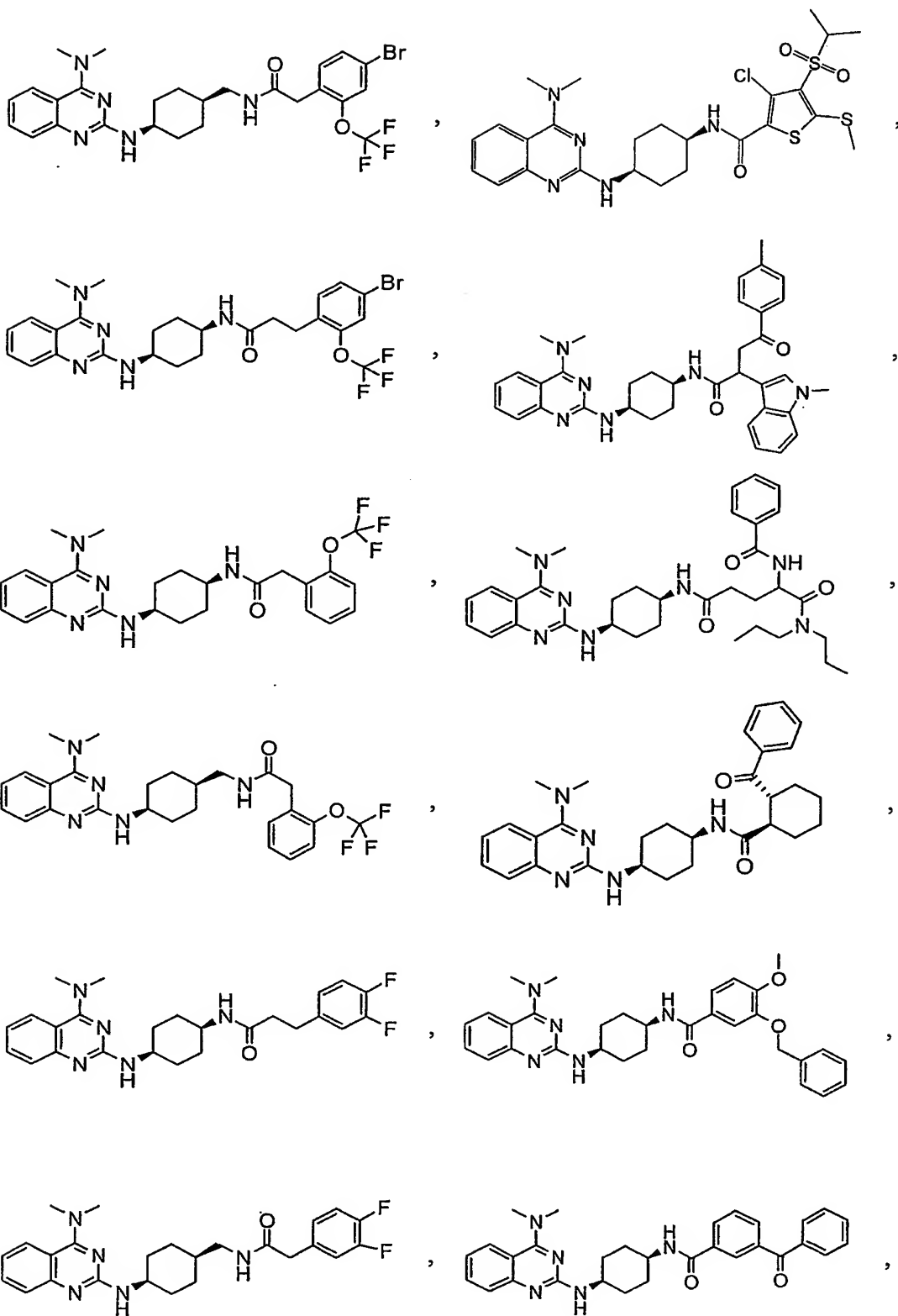
thienyl, 1,2,3-triazolyl, 1*H*-pyrrolyl, 2,3-dihydro-1-oxo-isoindolyl, 2,3-dihydro-benzofuryl, 2*H*-benzopyranyl, 2-oxo-benzopyranyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, imidazolyl, isoxazolyl, morpholino, morpholinyl, pyrazolyl, pyrimidyl, quinolyl, thiazolyl, tetrahydro-thienyl, benzofuranyl, or benzothiazolyl;

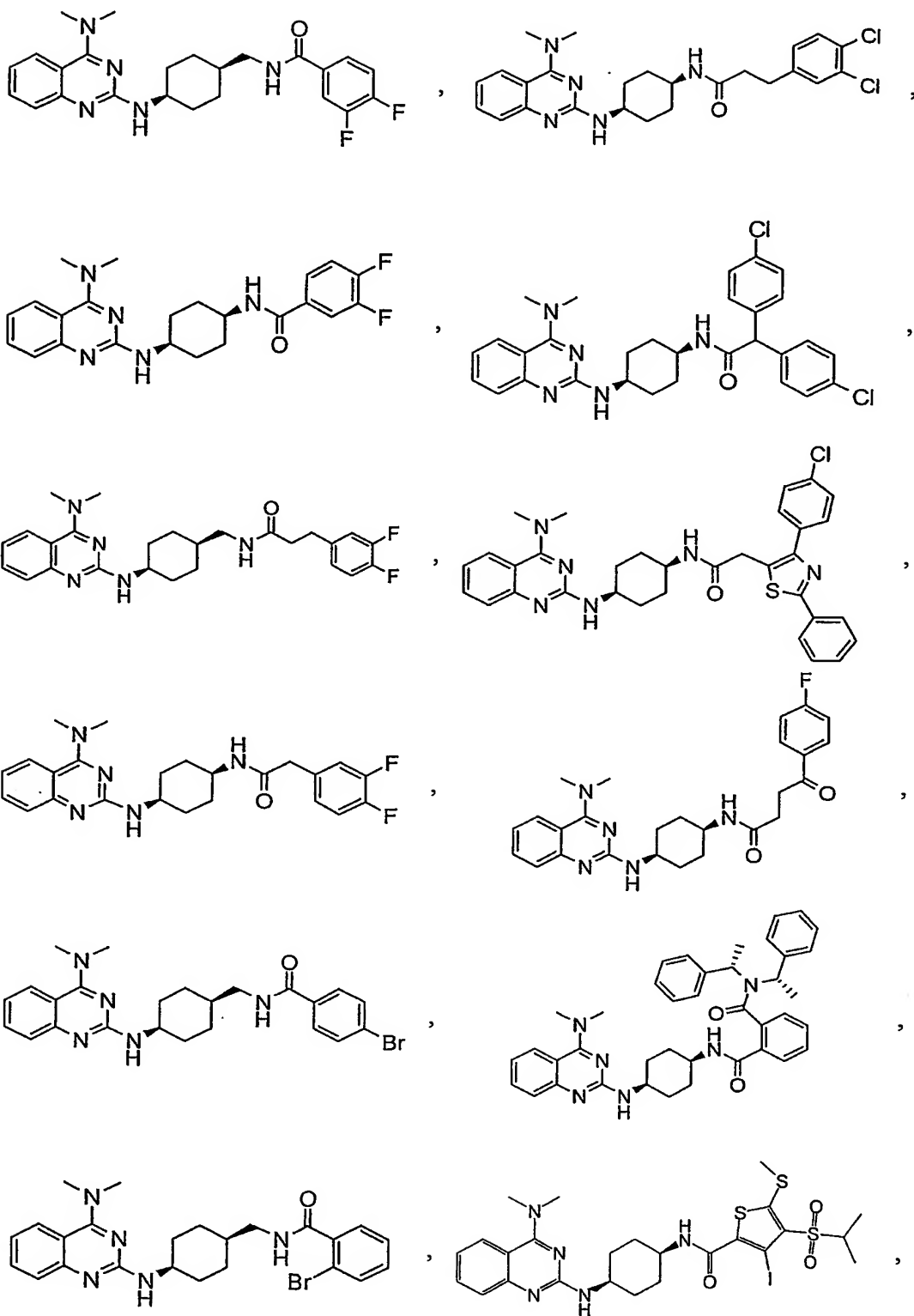
halogen is fluoro, chloro, bromo, or iodo;

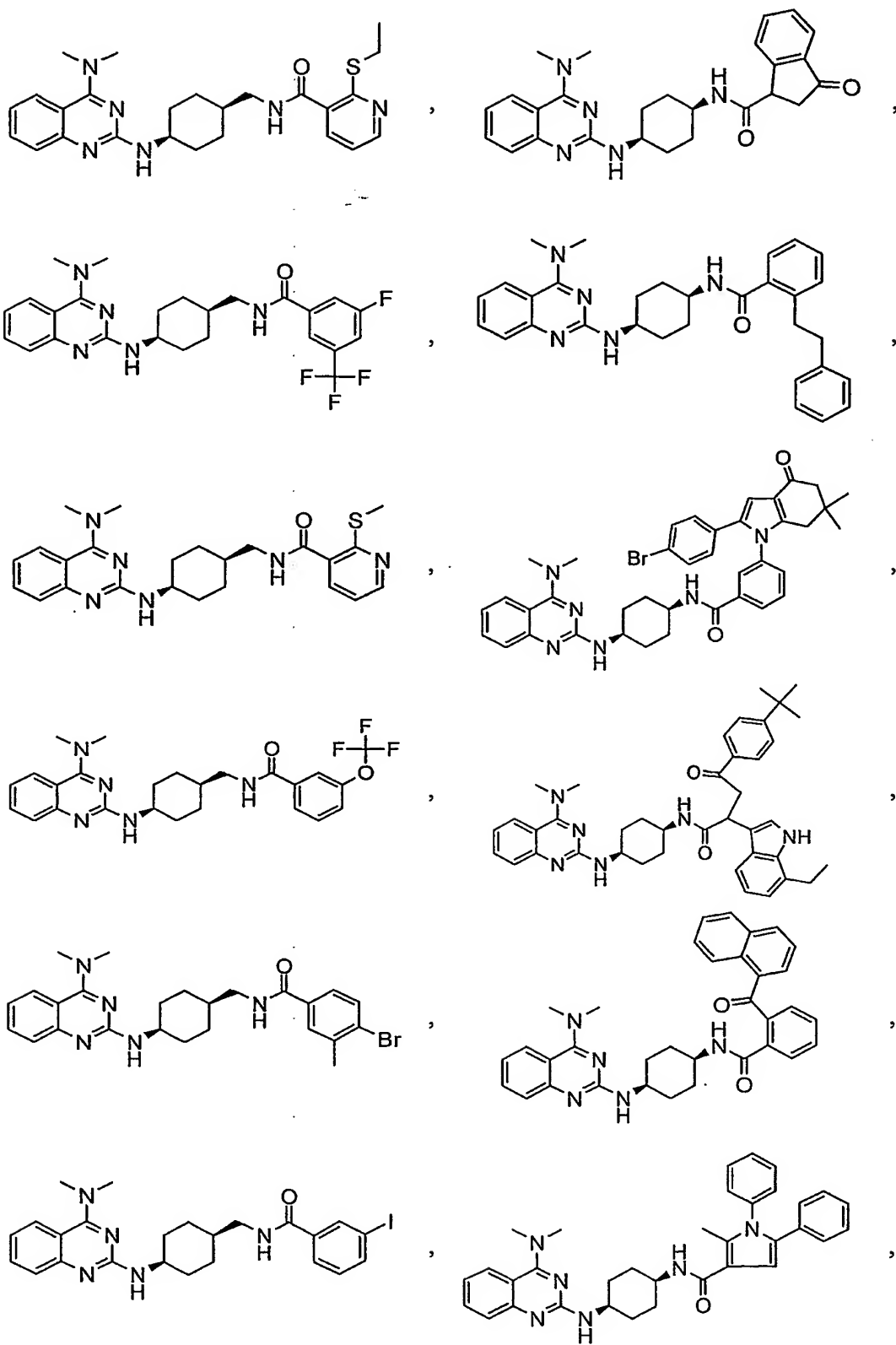
or a salt thereof.

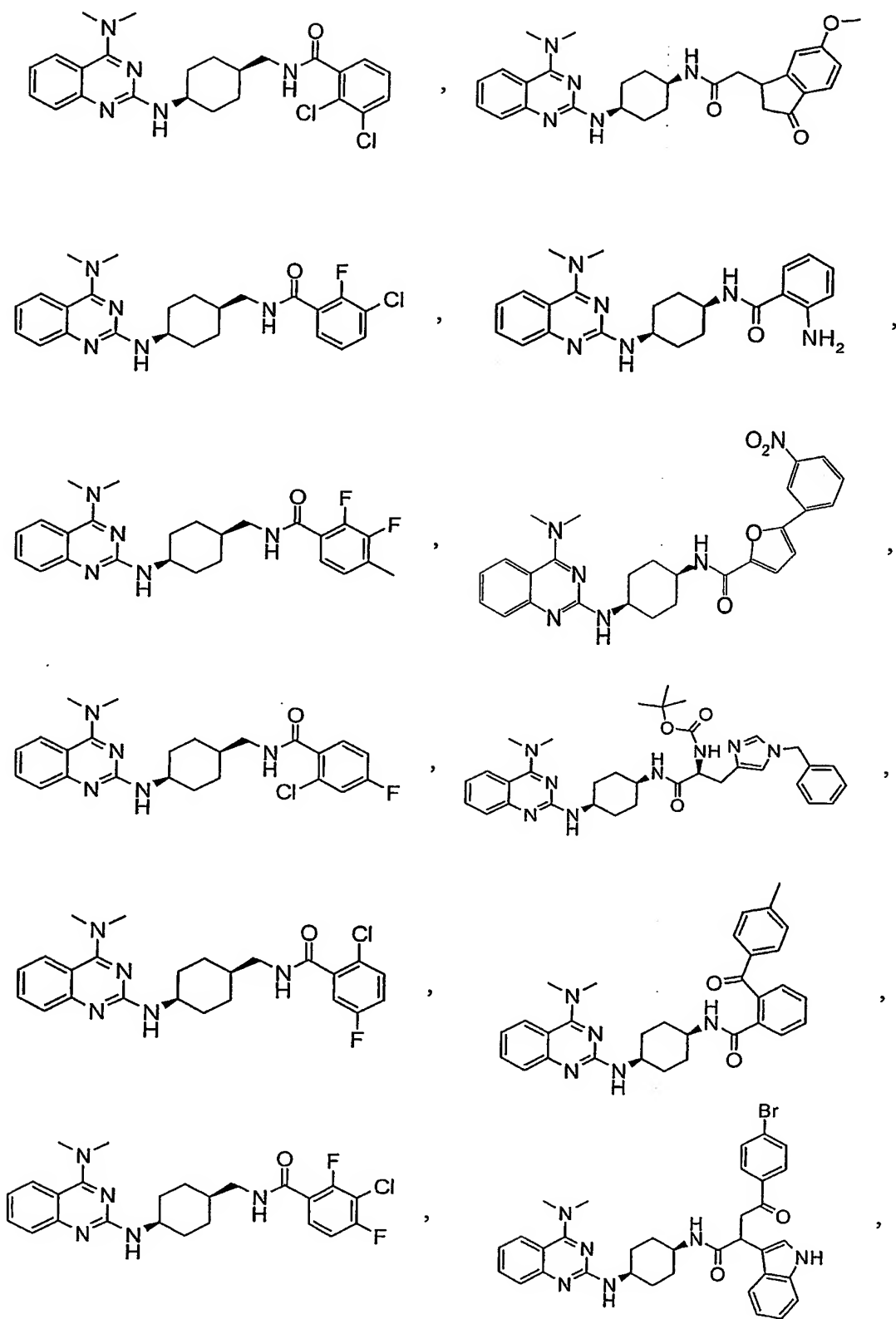
6. A compound according to claim 5 of Formua I selected from the group consisting of

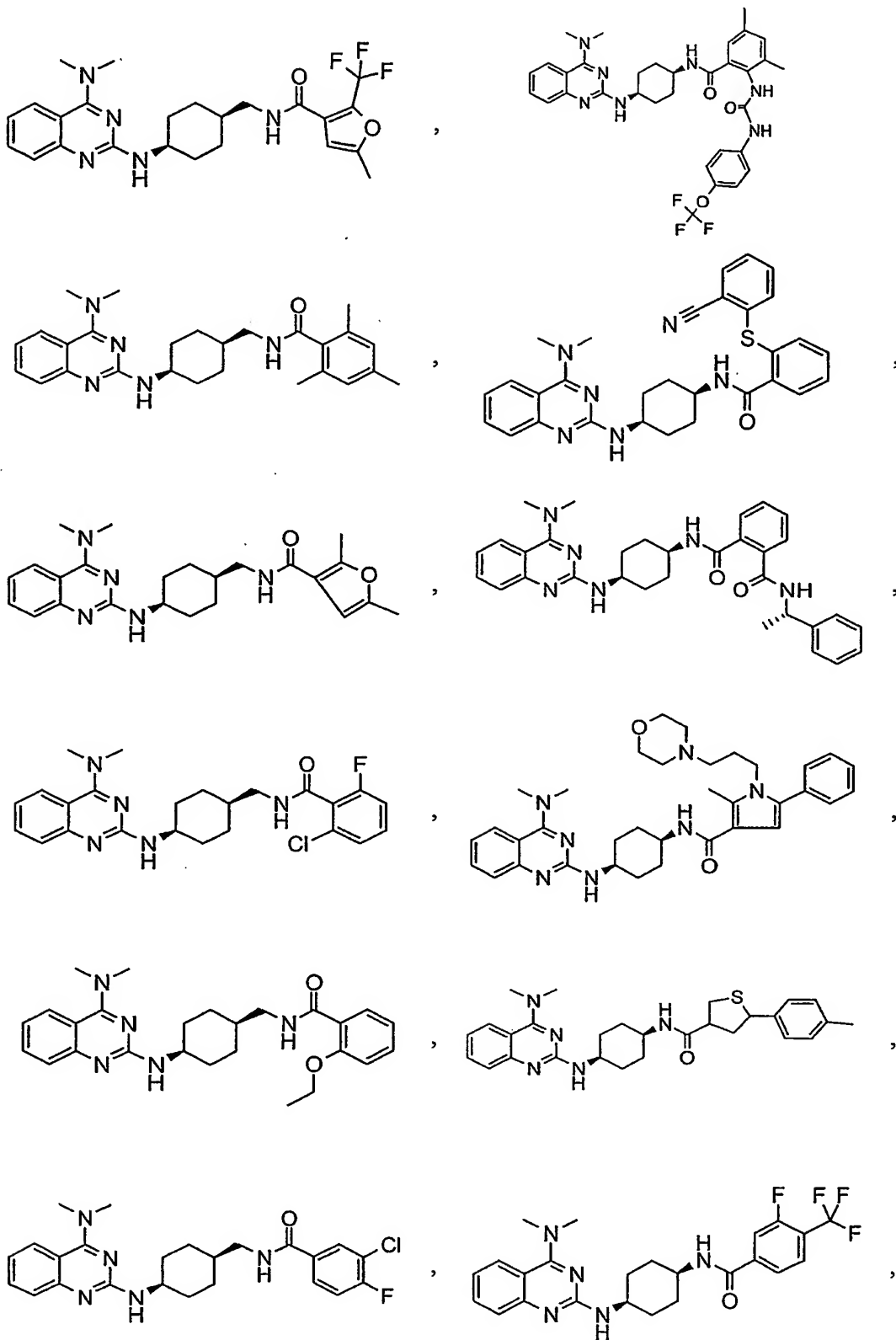


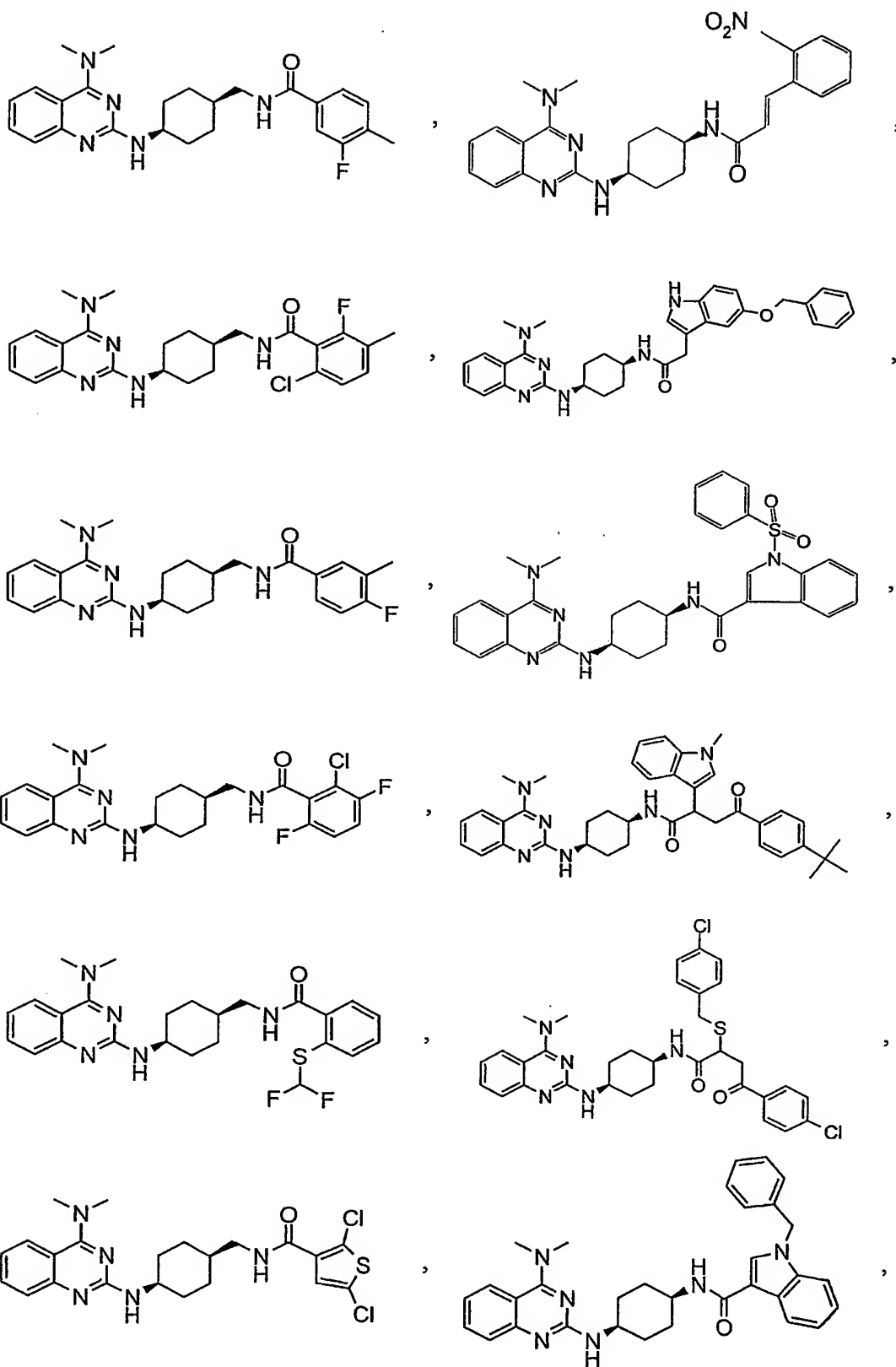


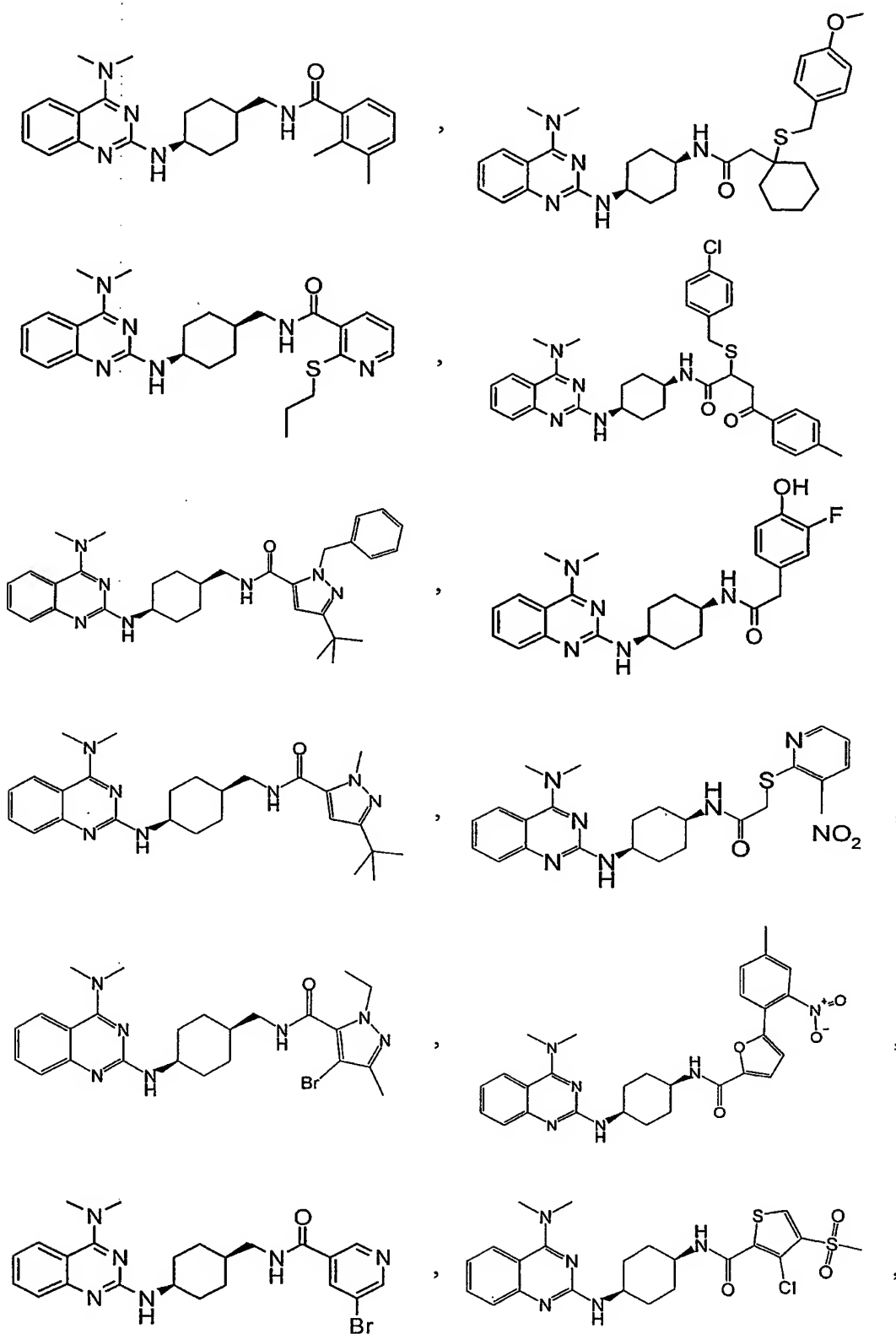


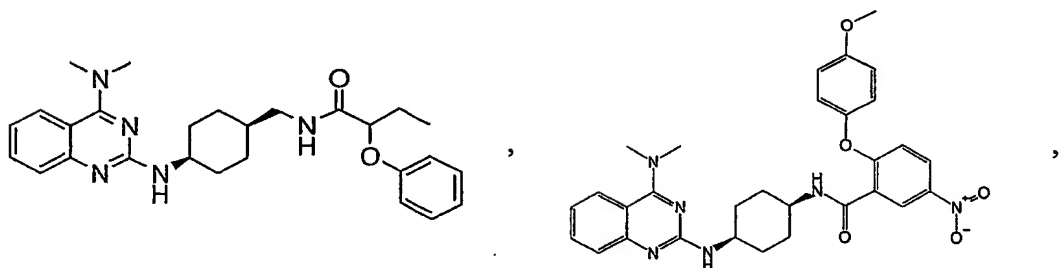
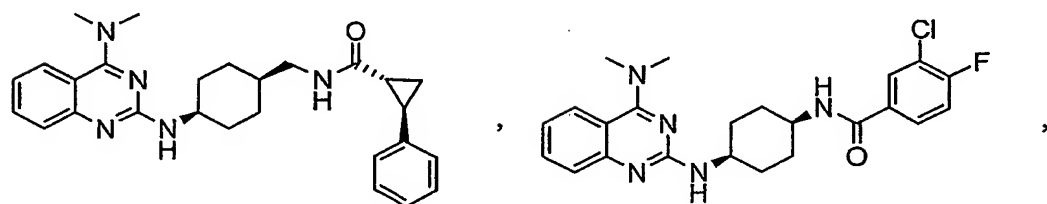
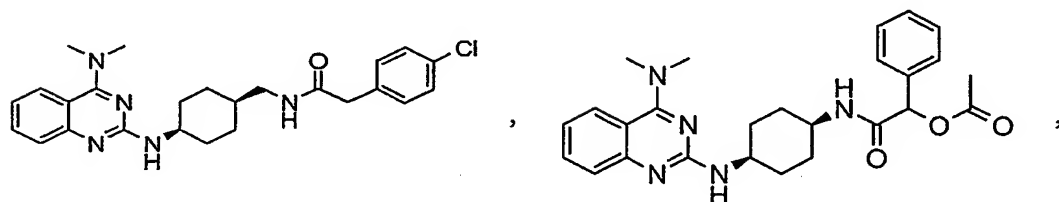
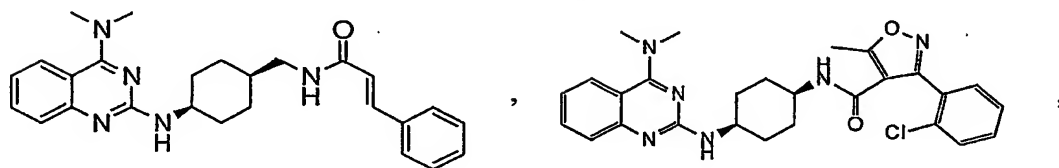
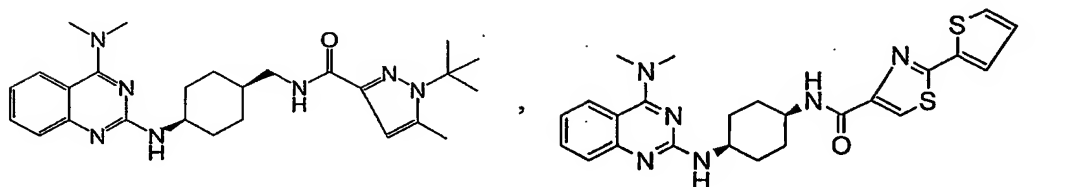
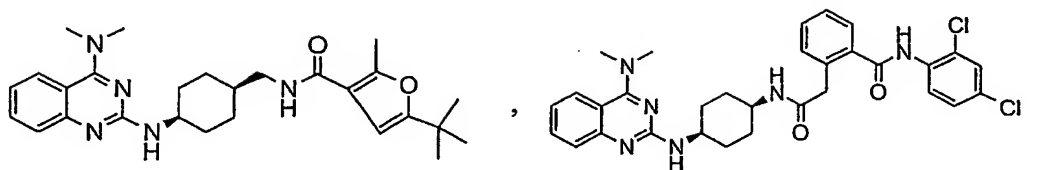


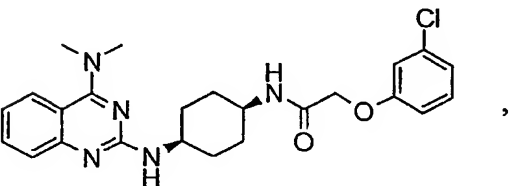
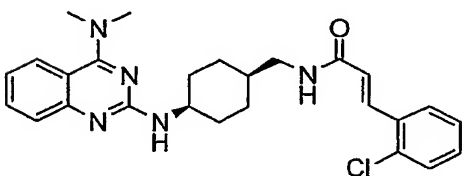
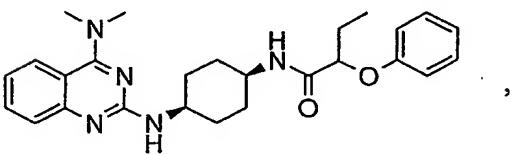
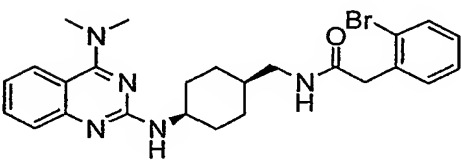
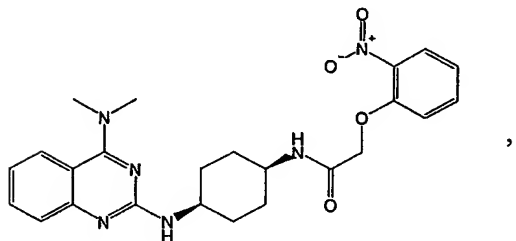
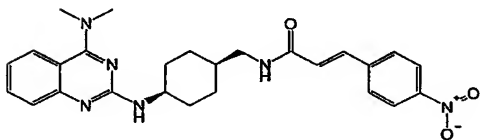
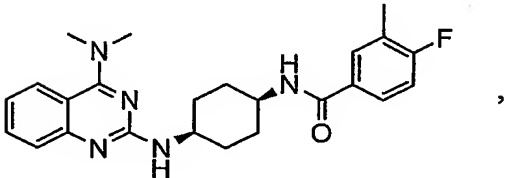
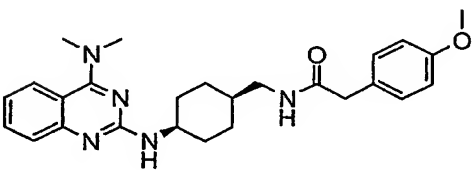
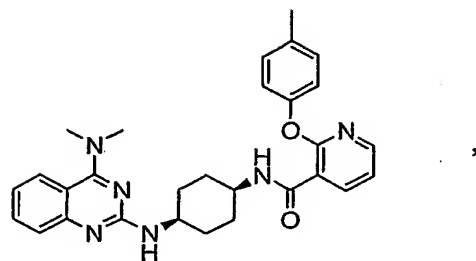
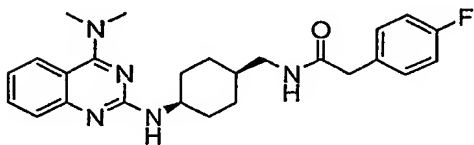
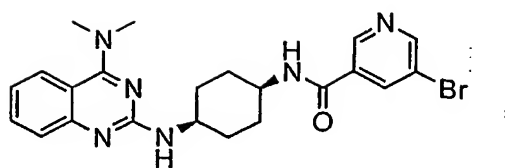
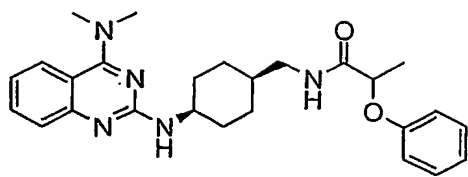


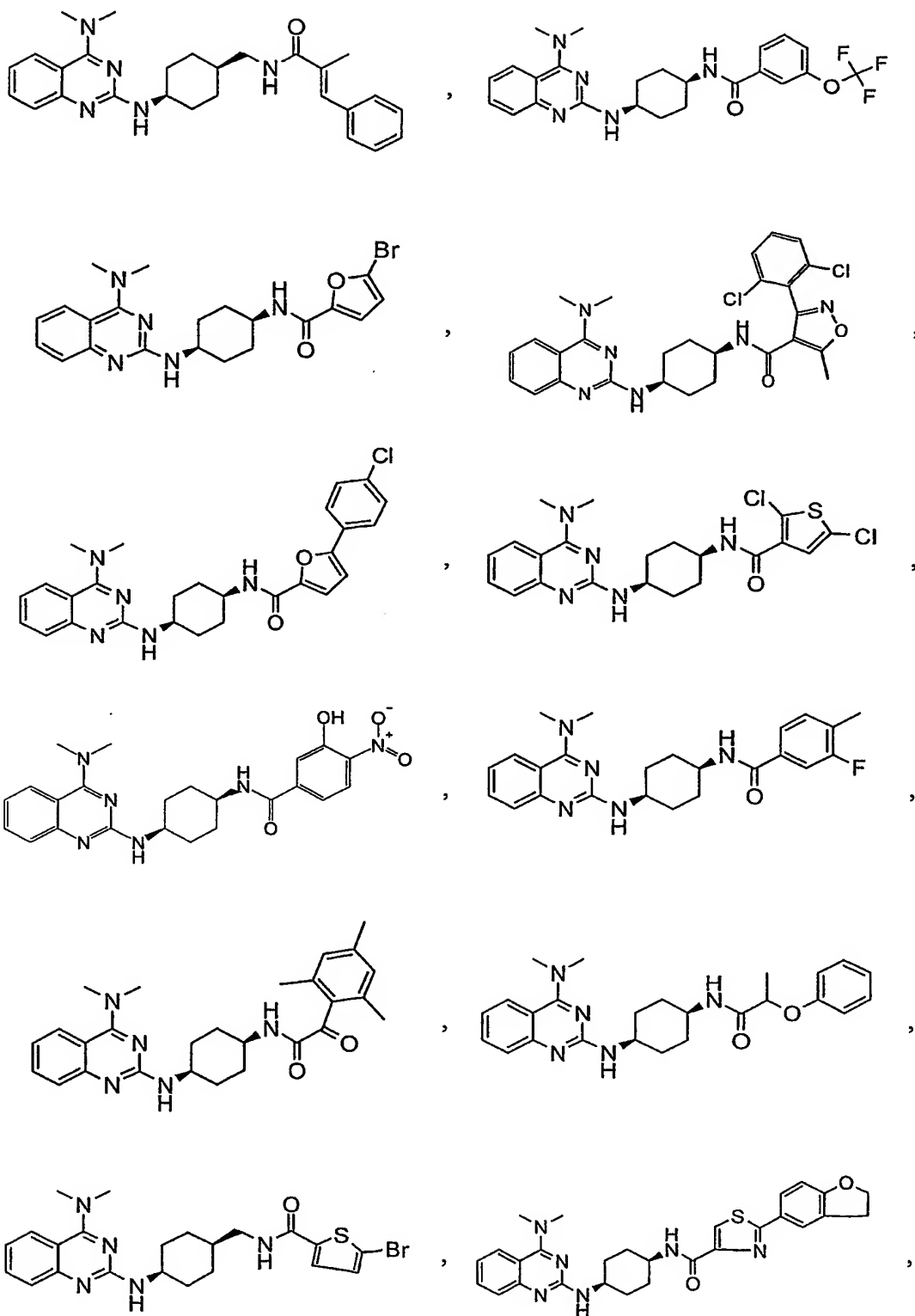


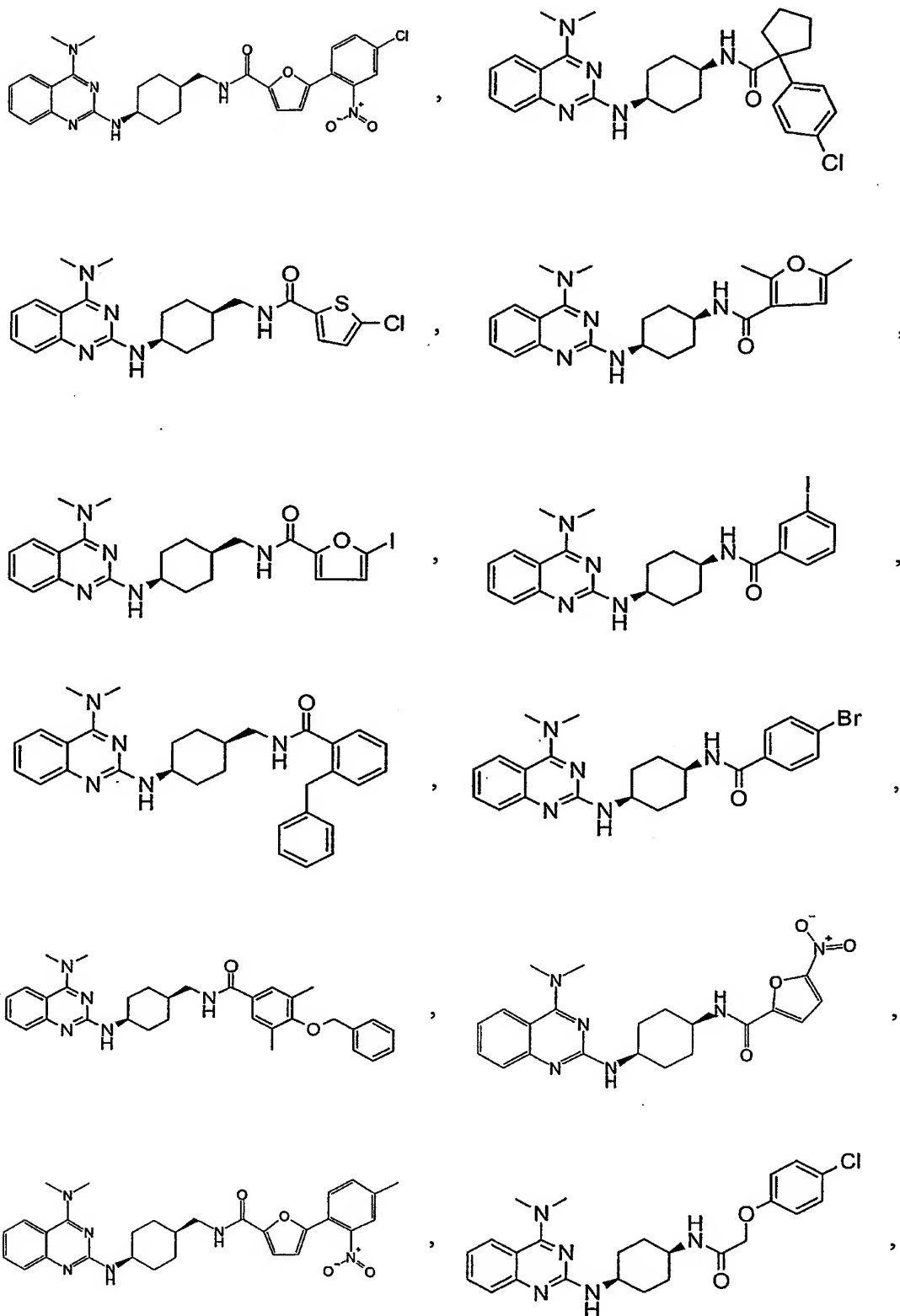


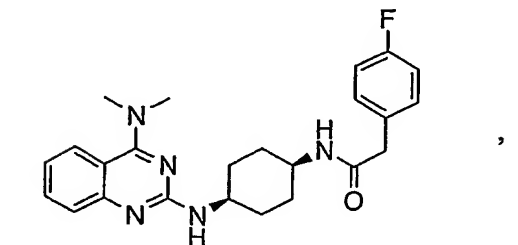
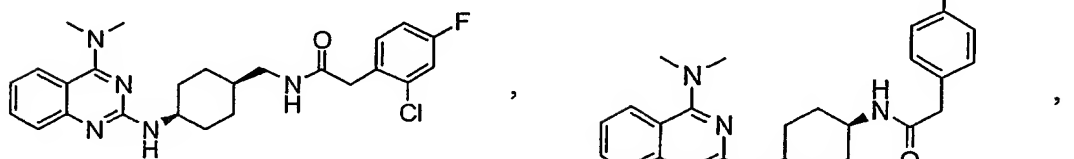
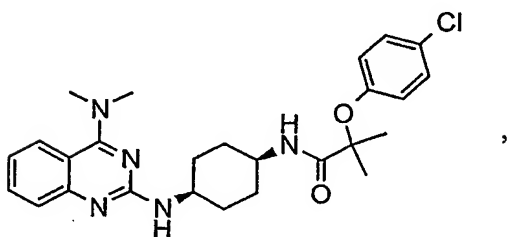
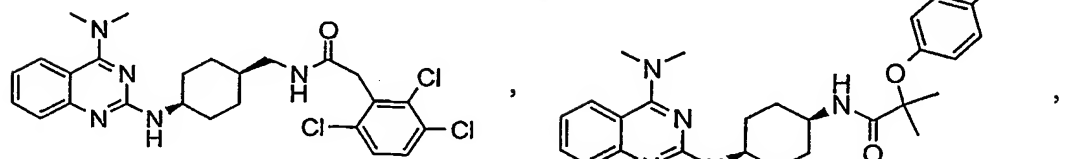
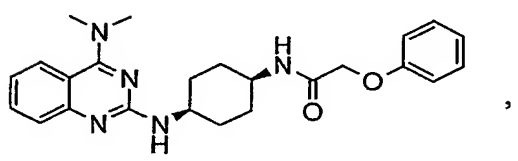
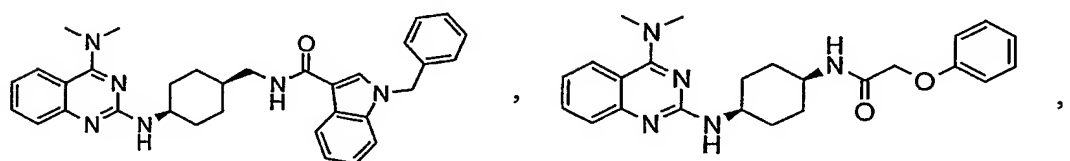
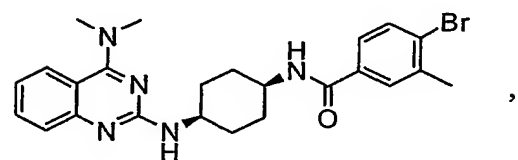
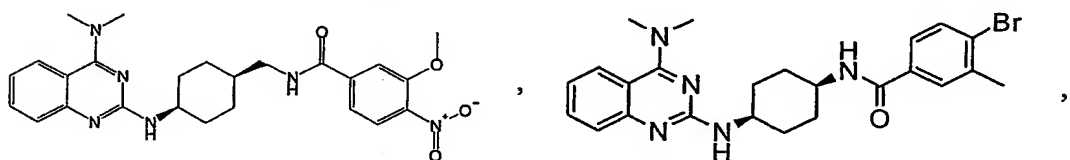
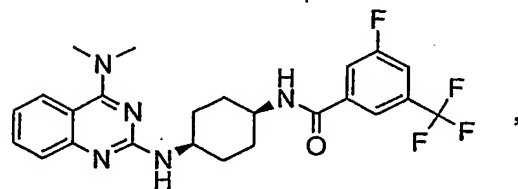
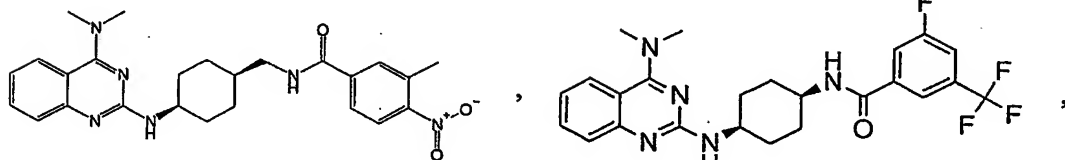
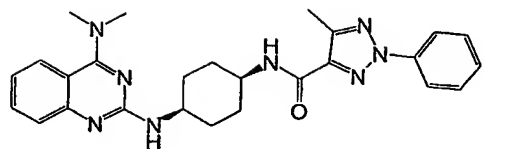
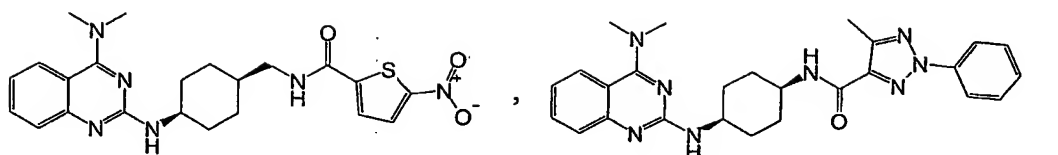


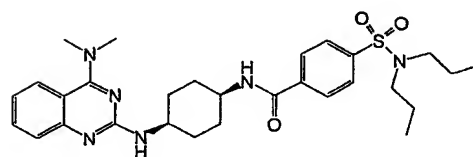
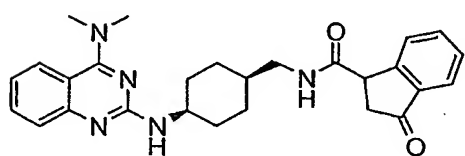
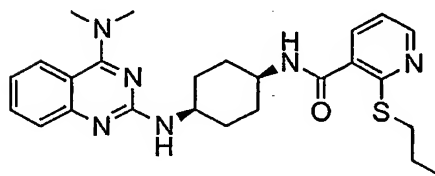
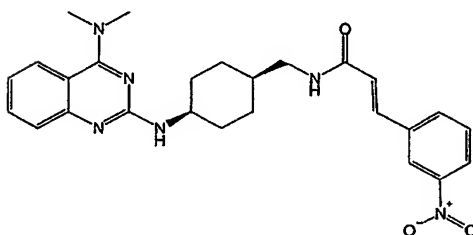
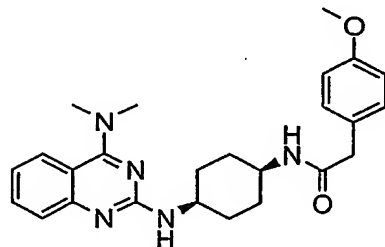
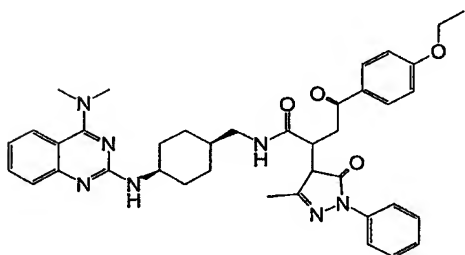
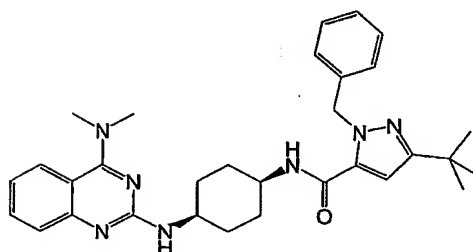
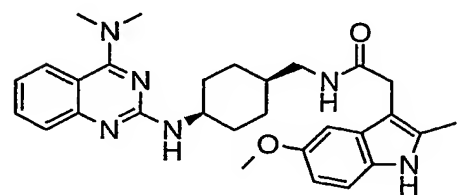
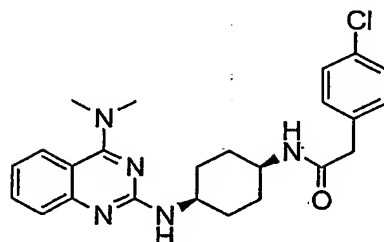
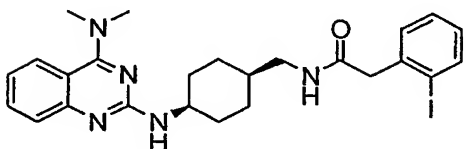
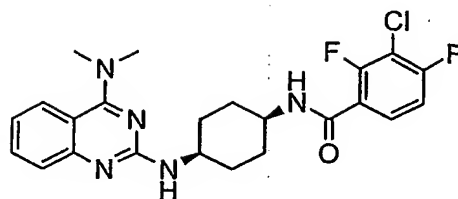
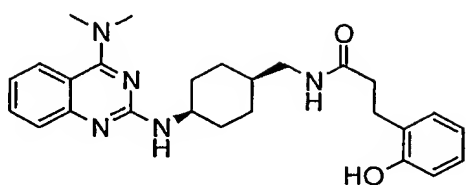


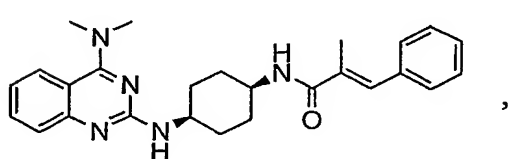
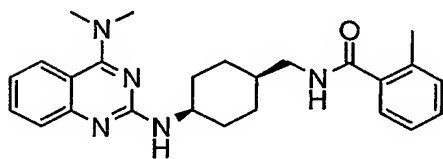
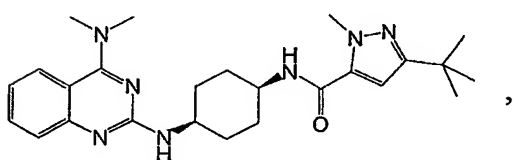
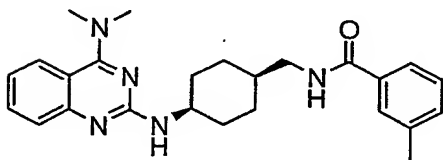
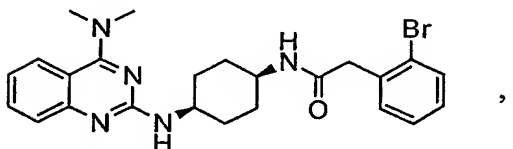
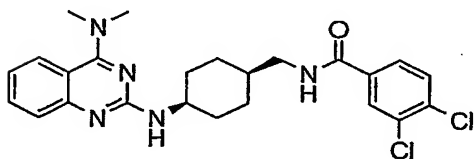
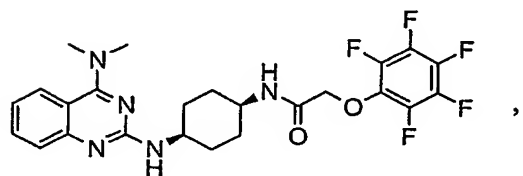
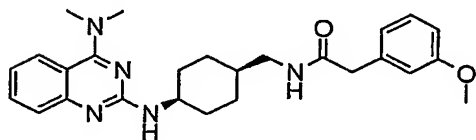
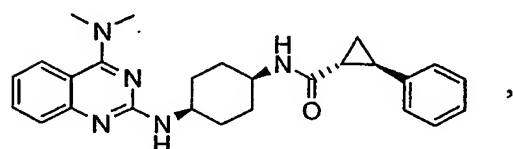
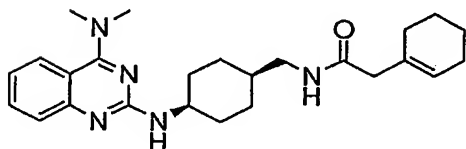
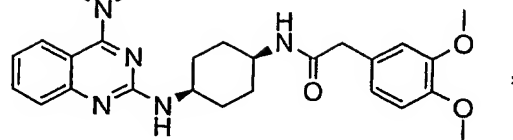
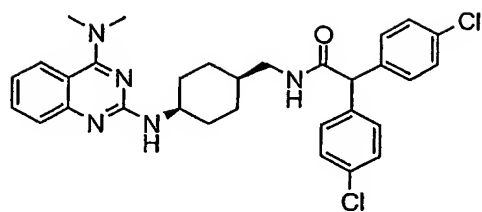


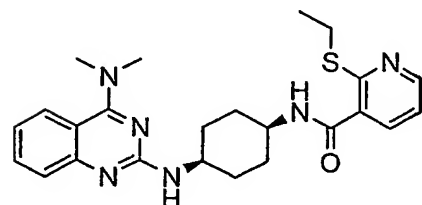
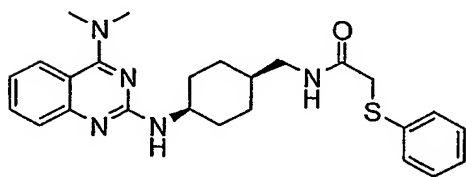
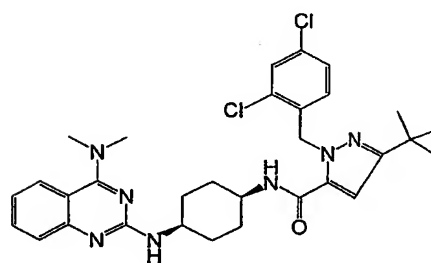
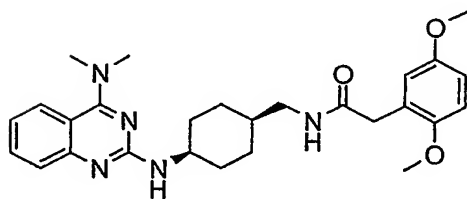
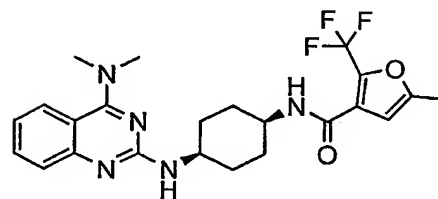
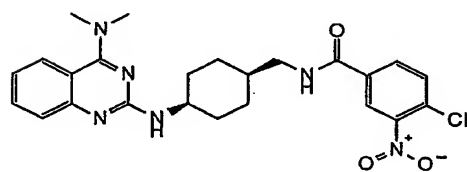
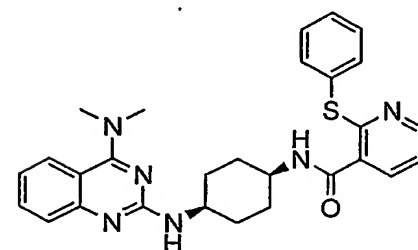
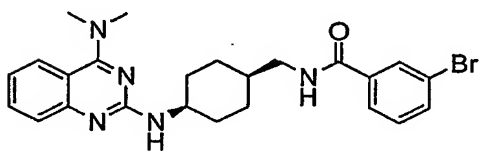
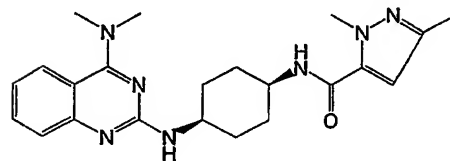
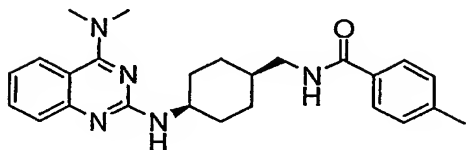
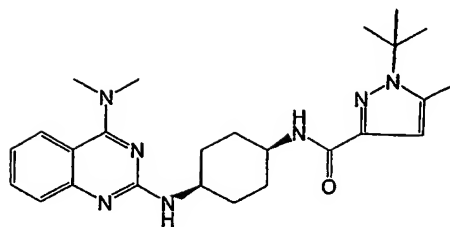
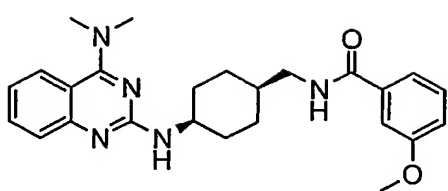


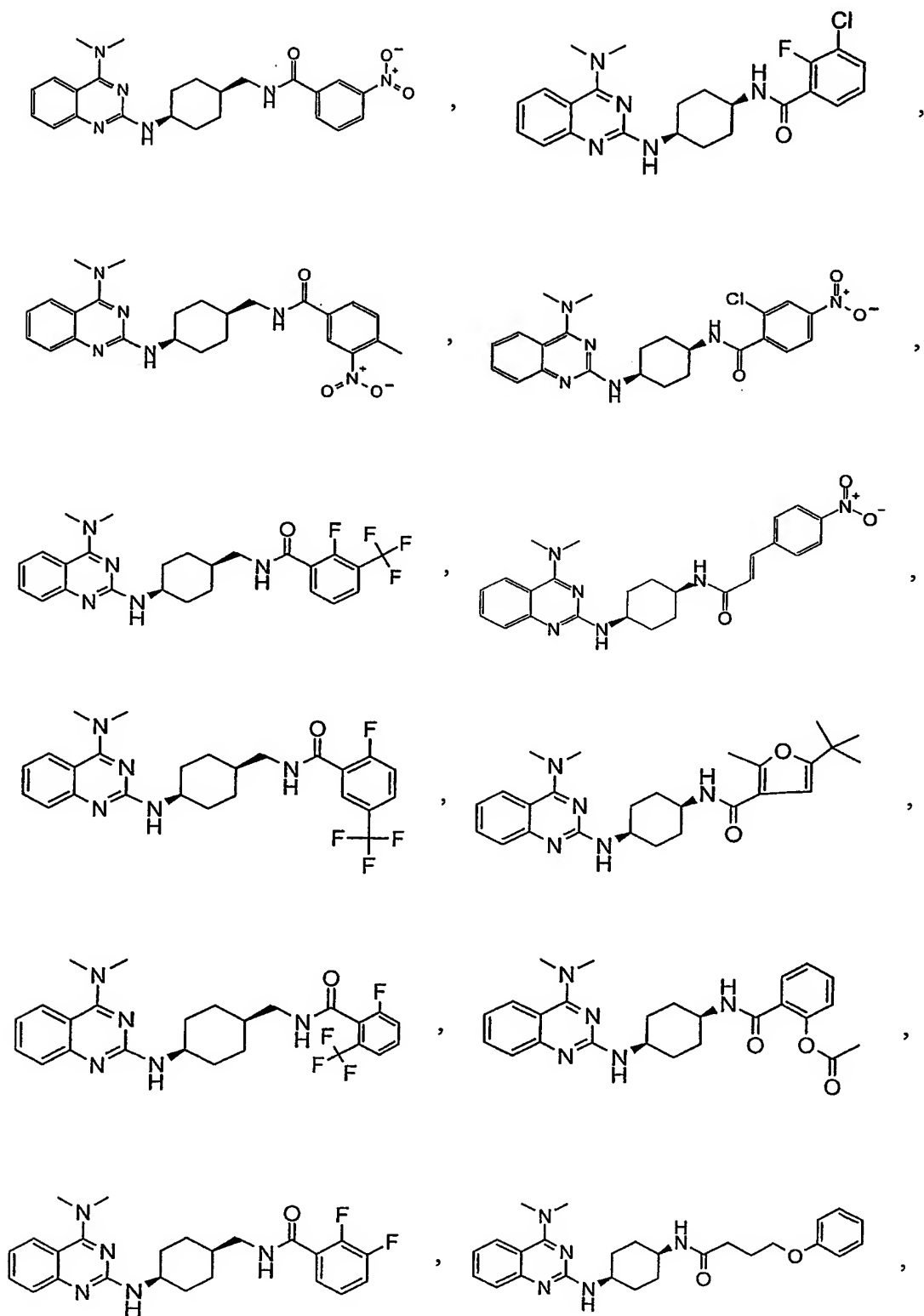


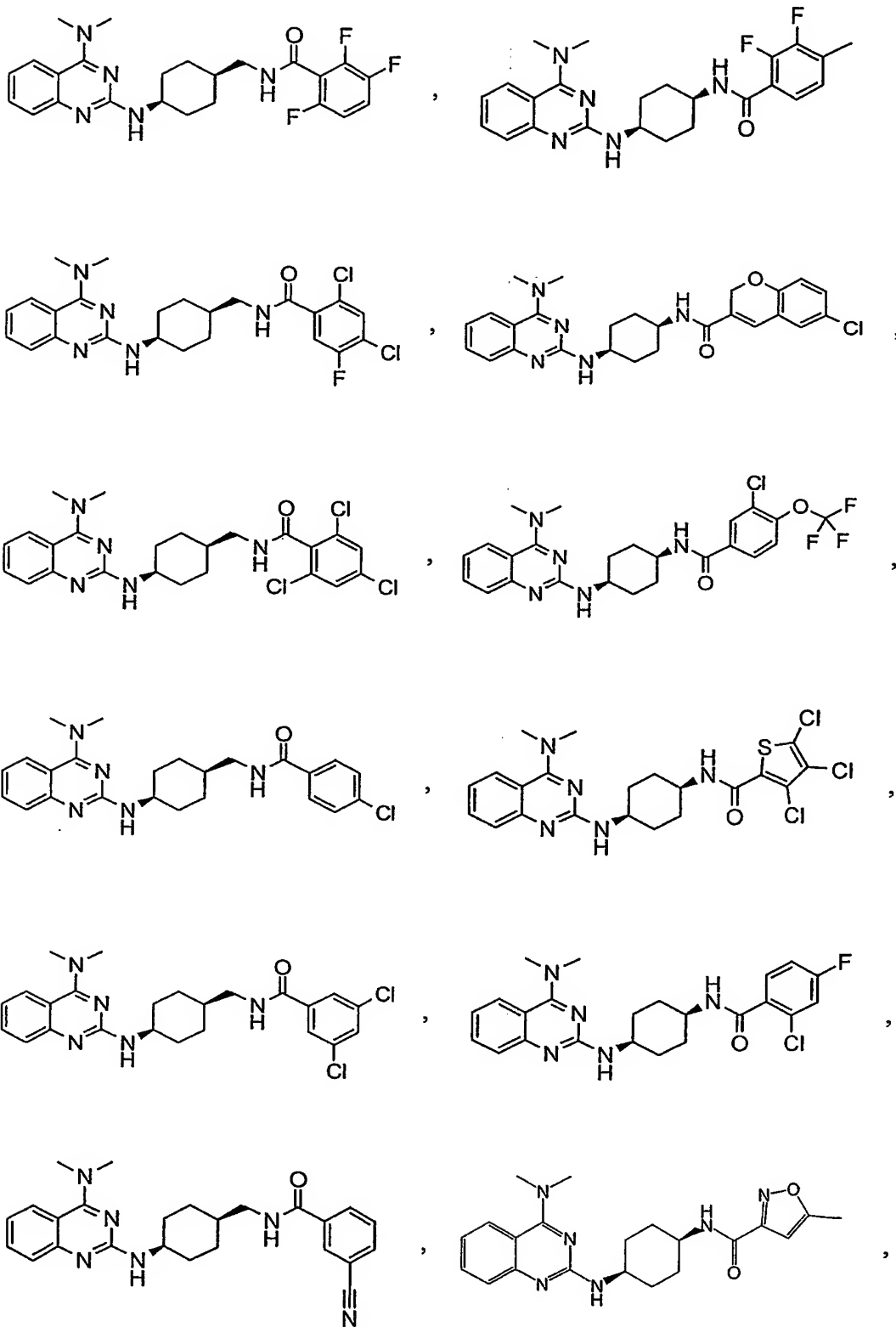


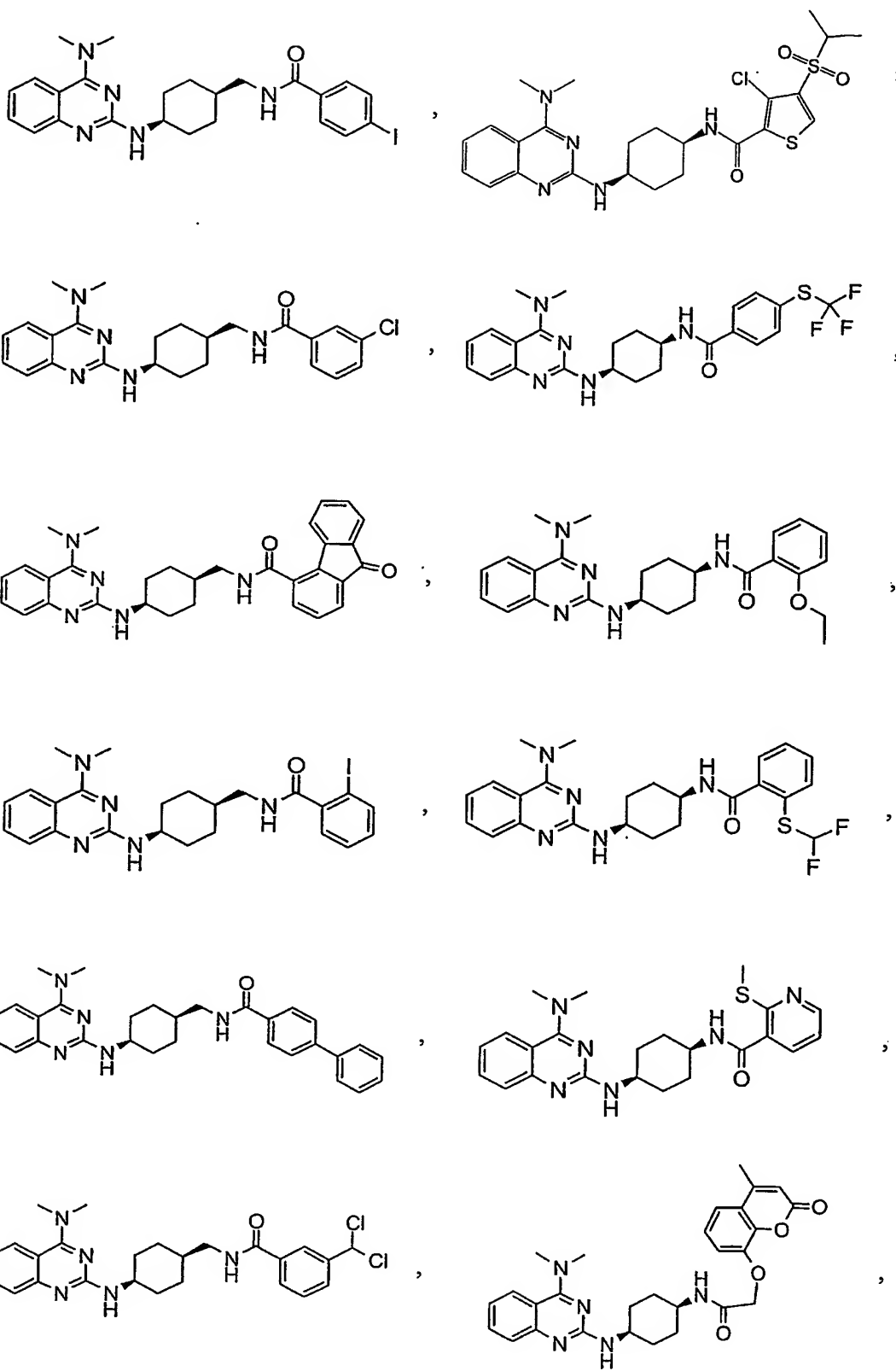


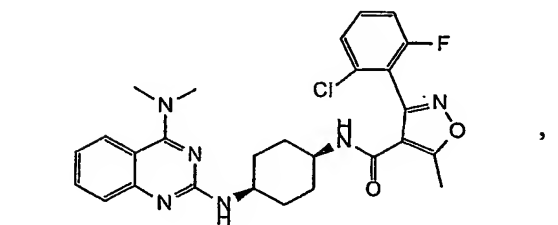
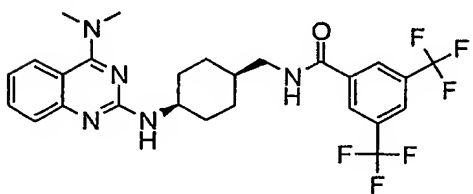
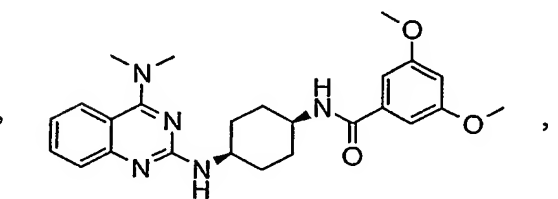
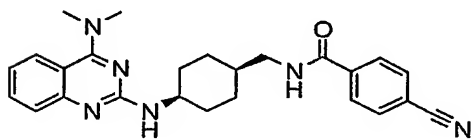
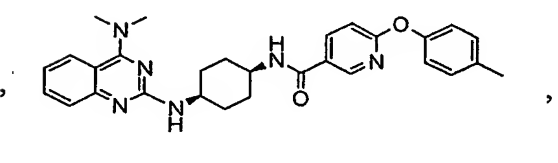
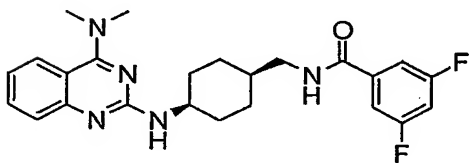
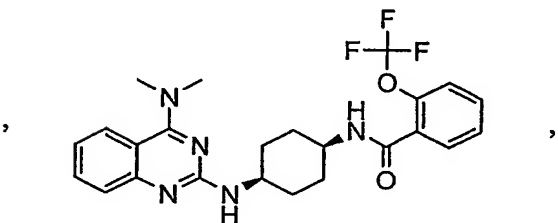
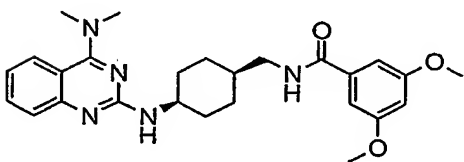
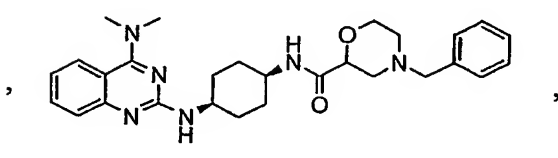
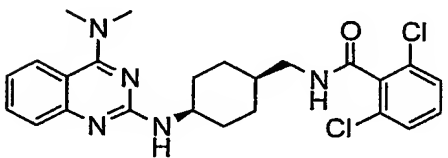
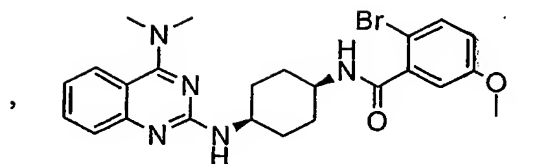
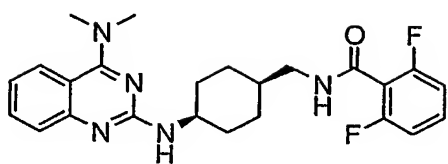


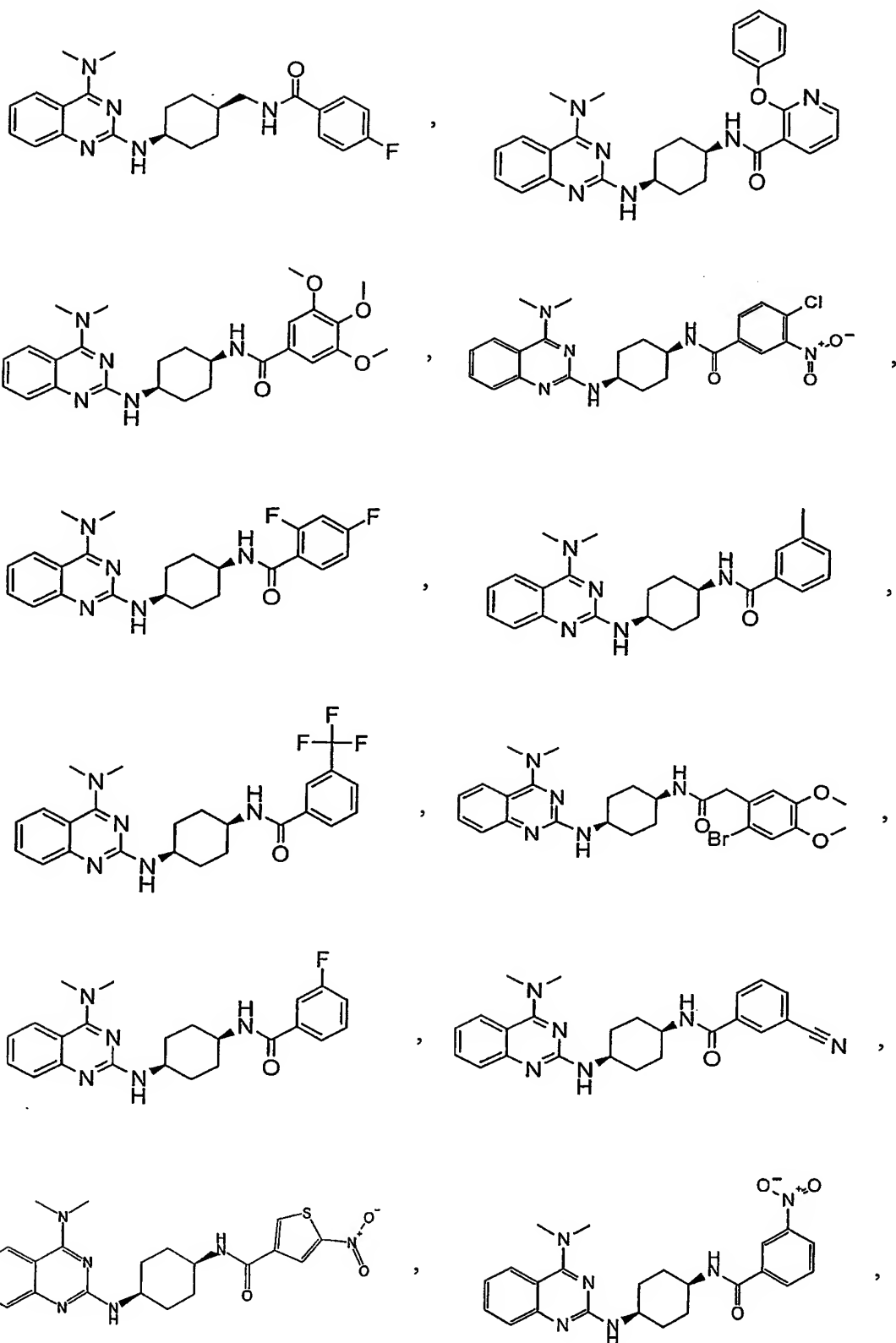


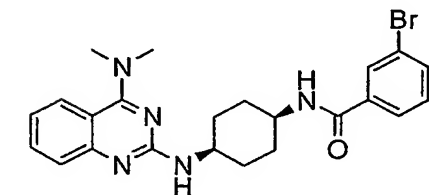
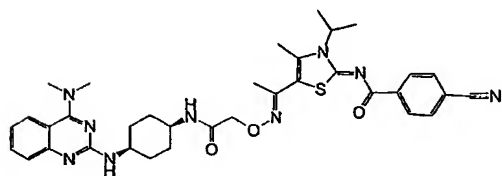
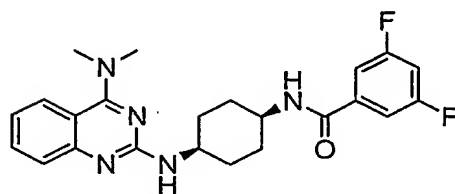
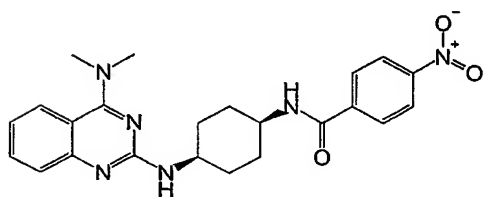
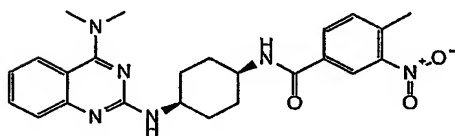
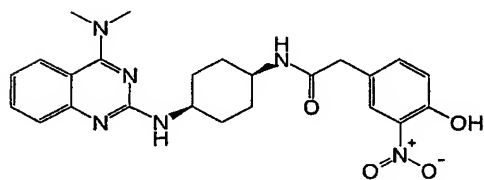
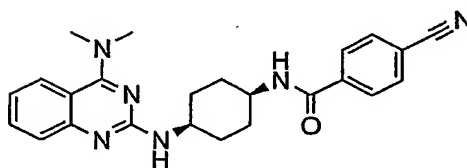
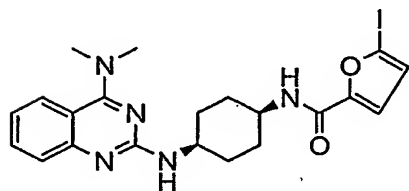
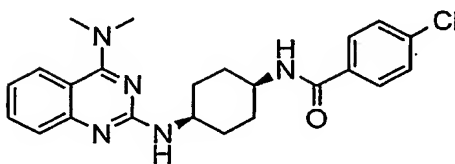
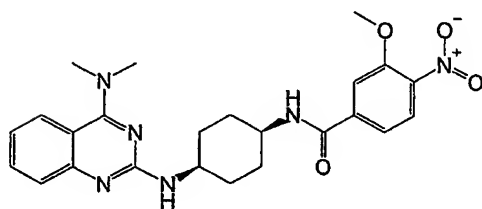
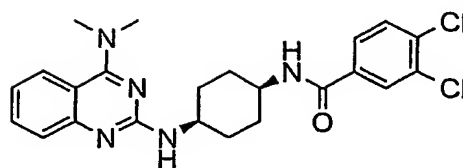
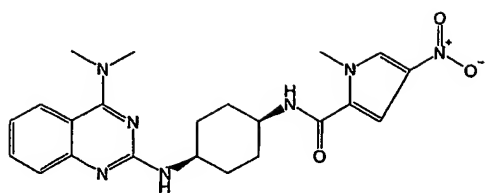


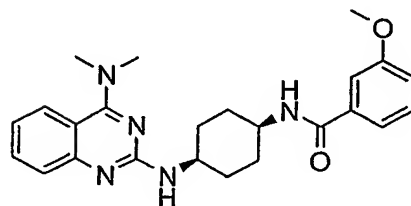
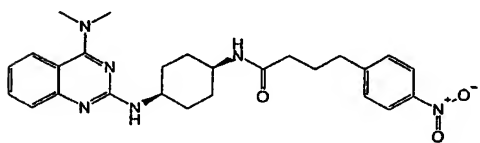
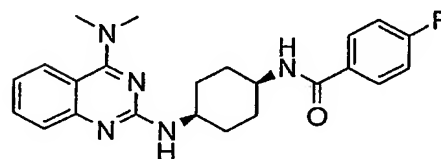
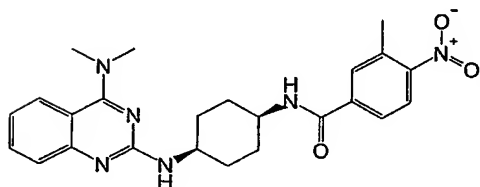
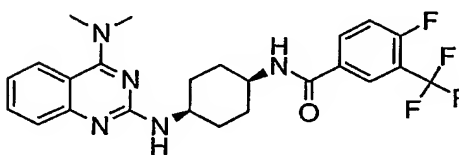
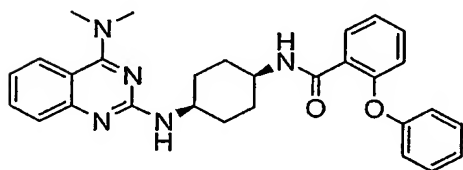
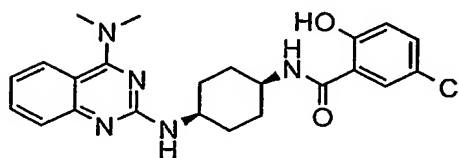
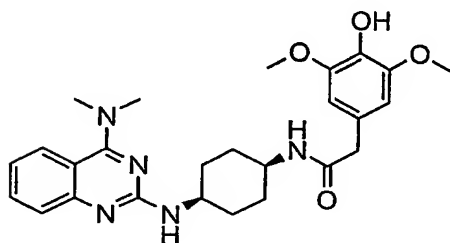
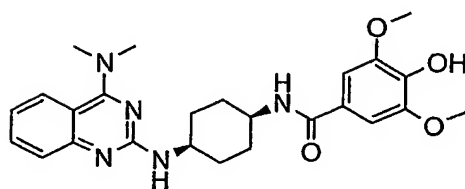
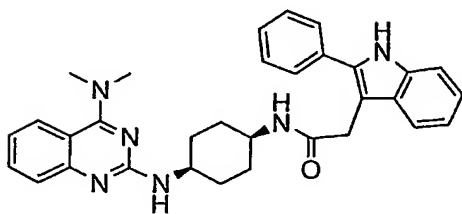
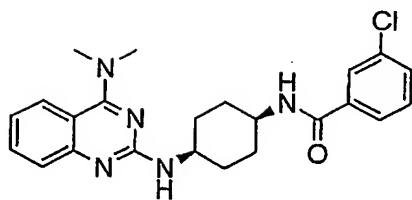
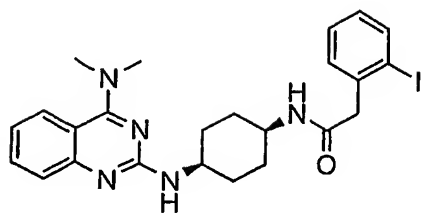


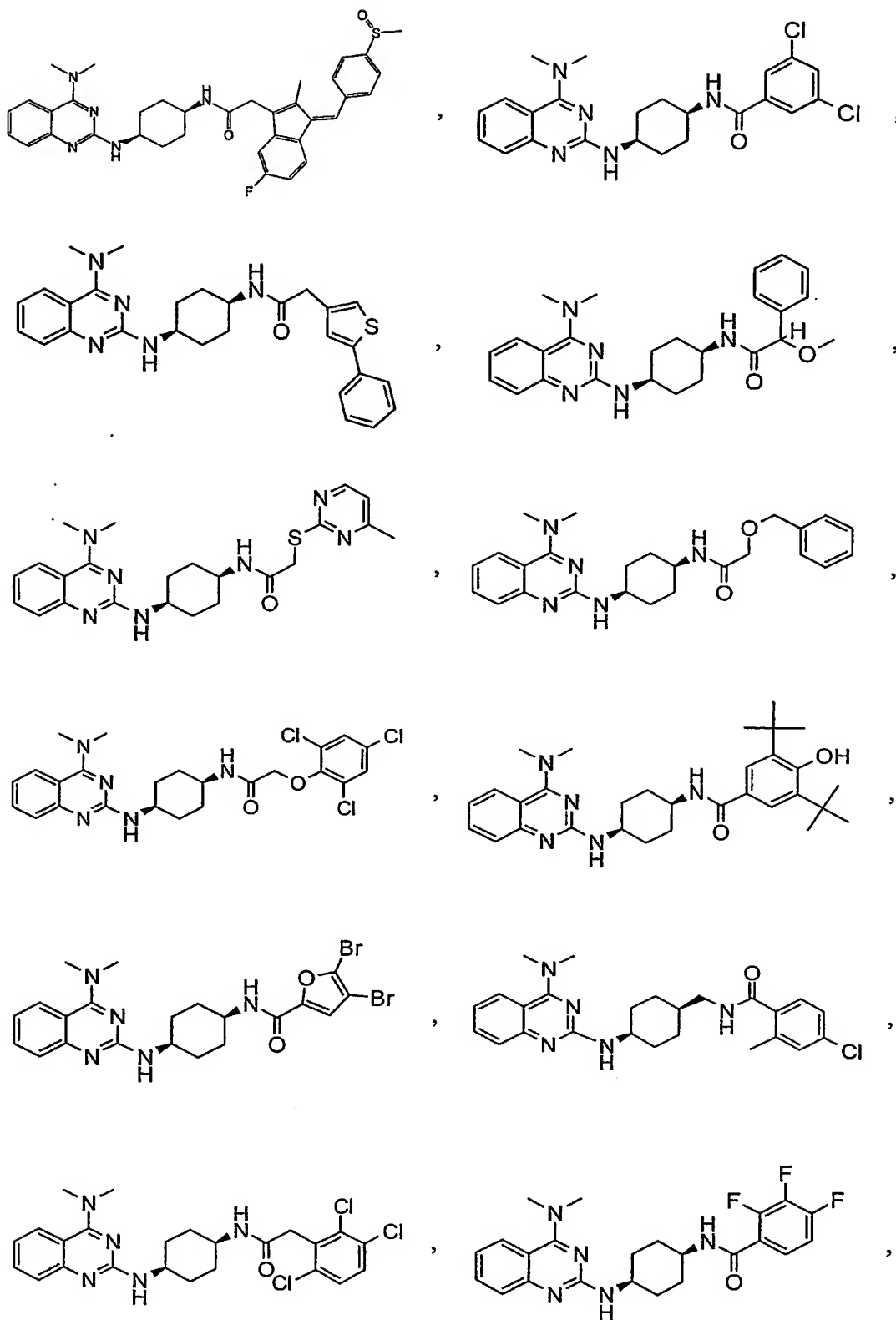


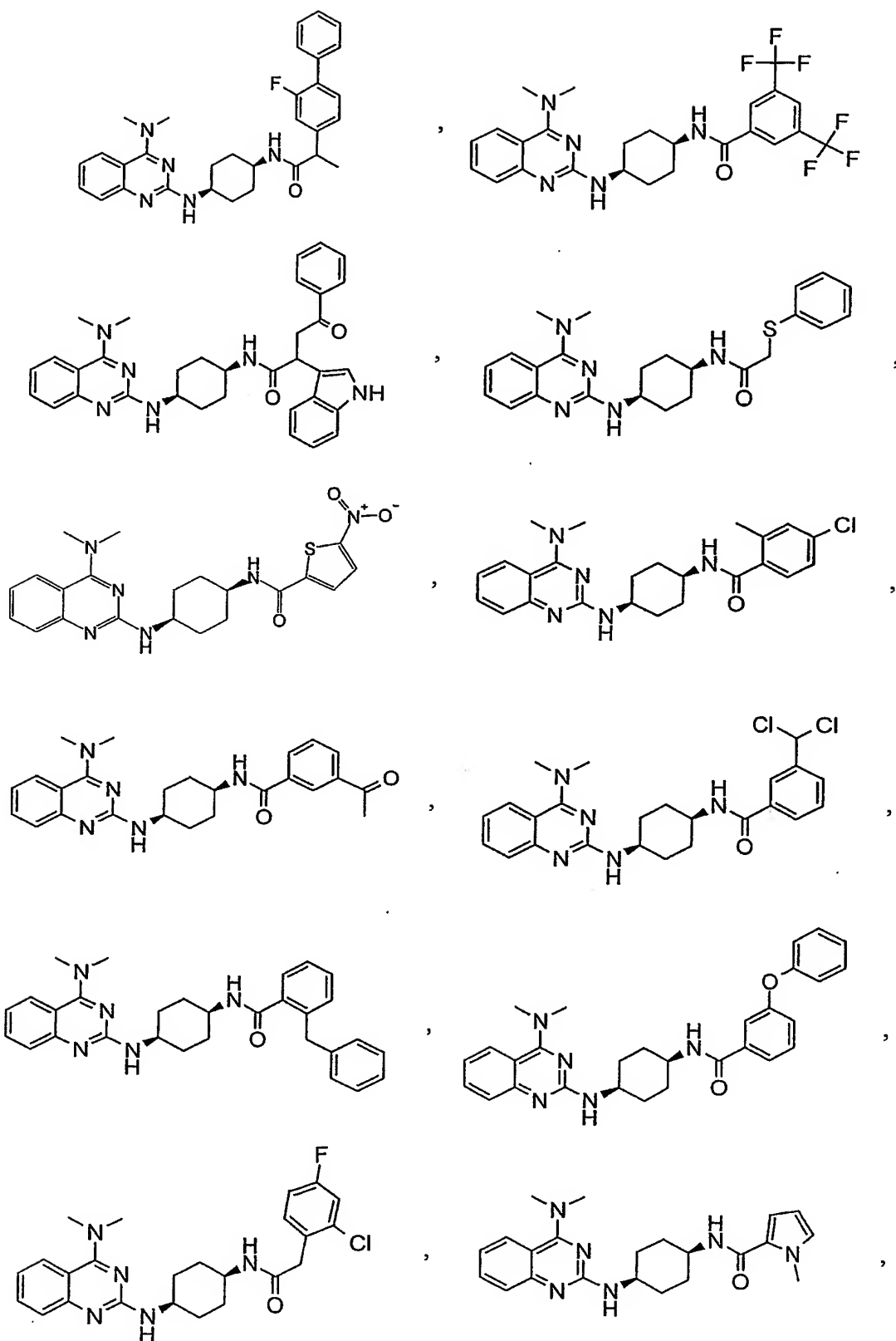


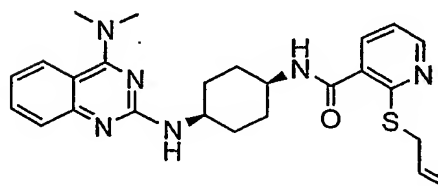
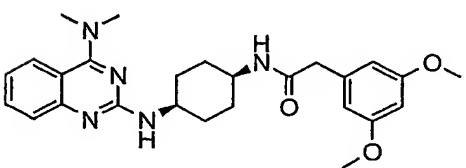
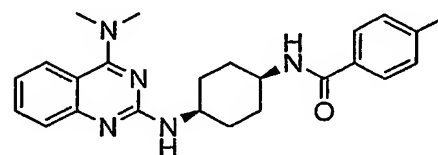
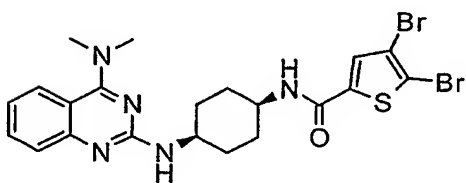
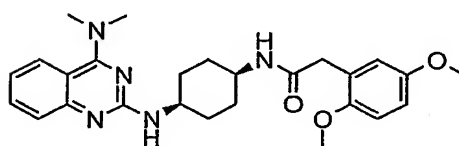
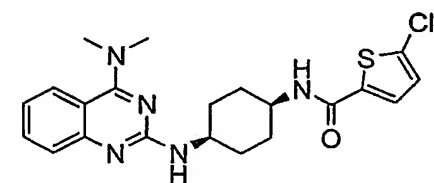
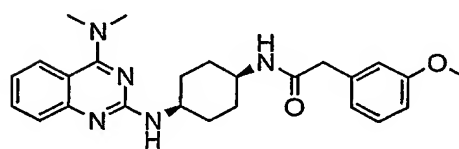
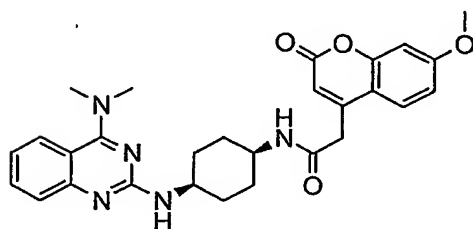
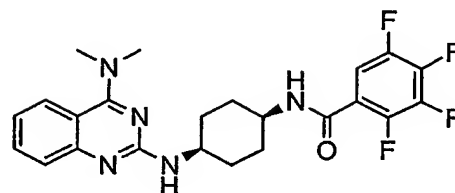
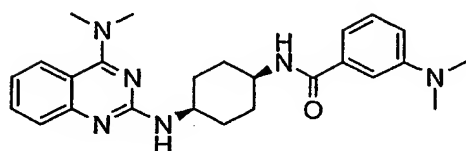
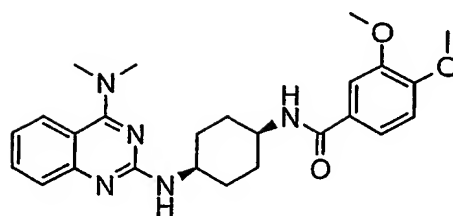
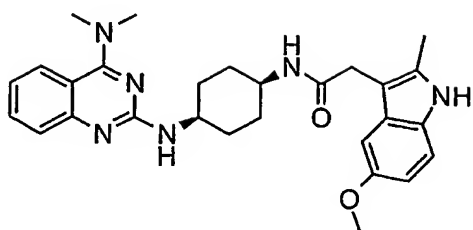


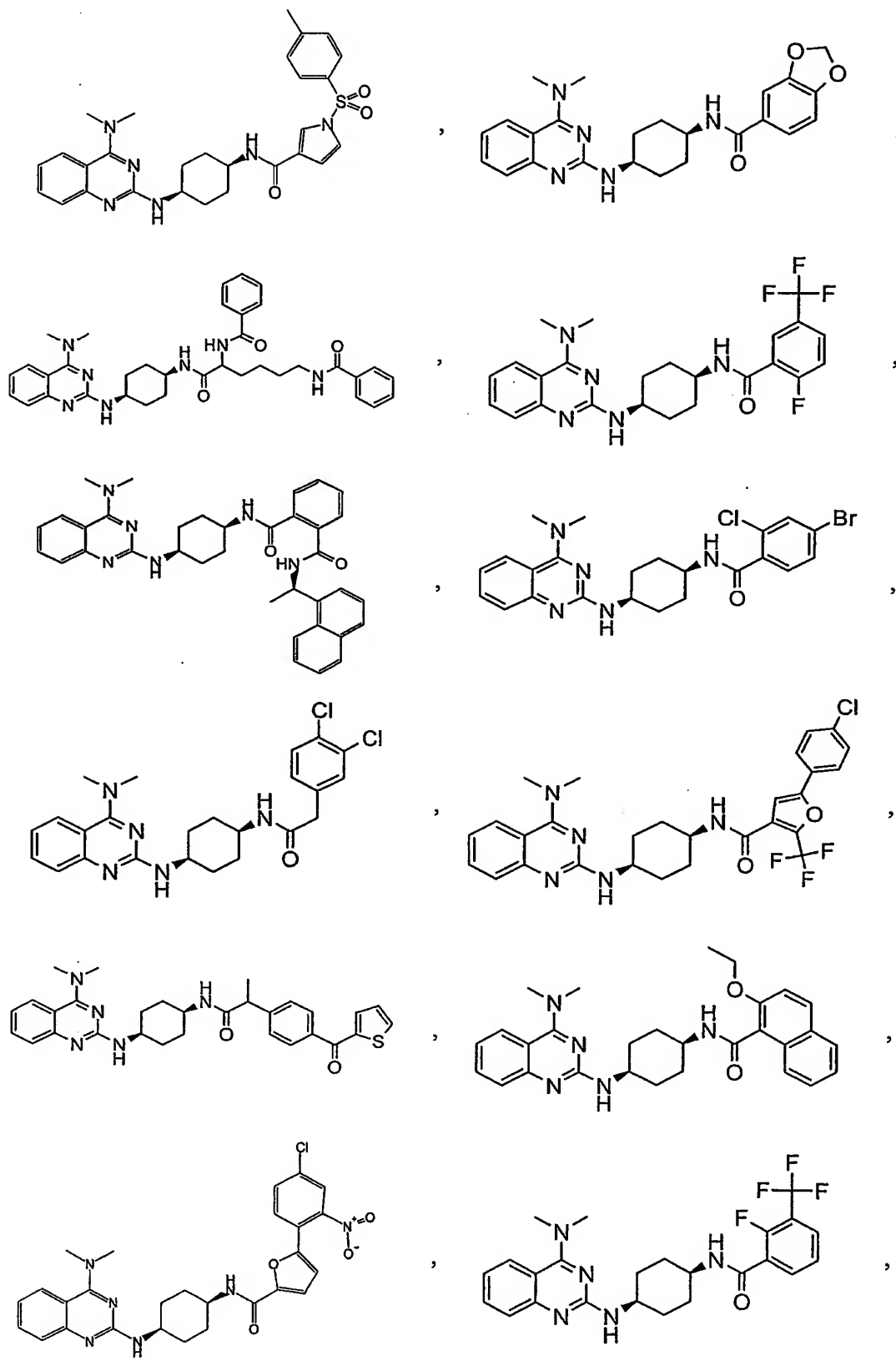


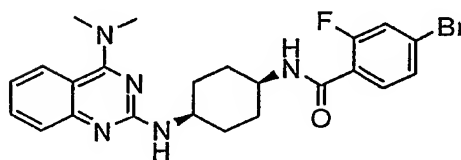
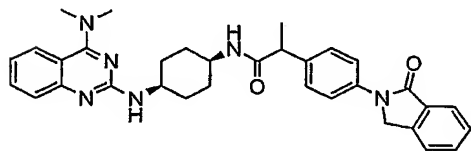
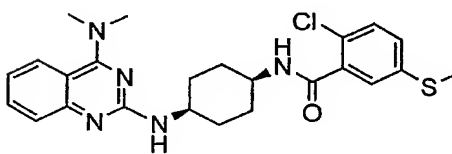
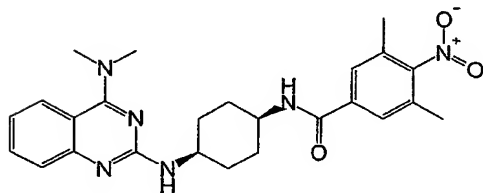
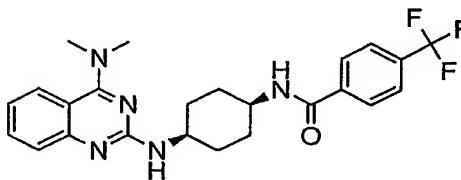
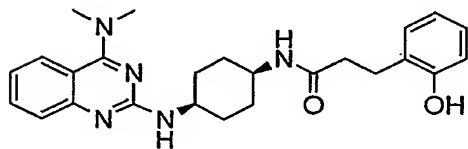
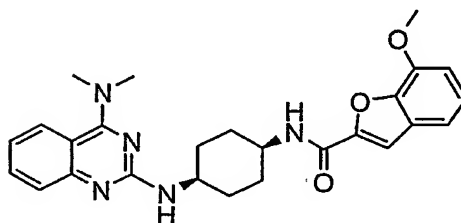
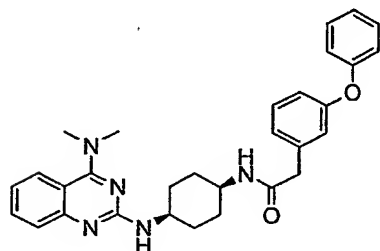
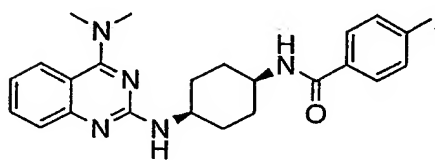
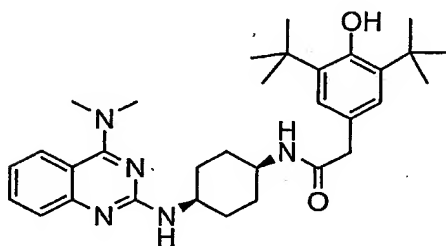
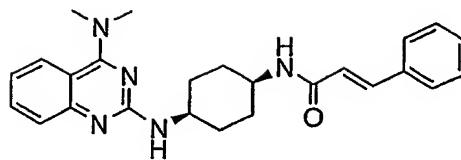
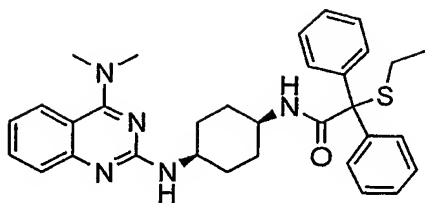


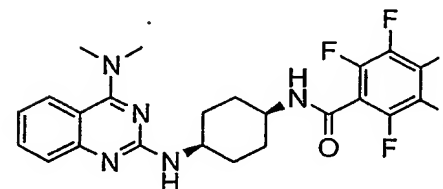
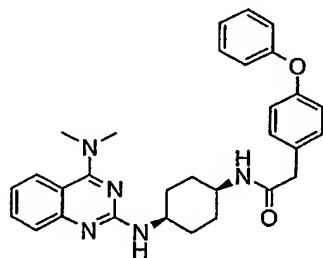
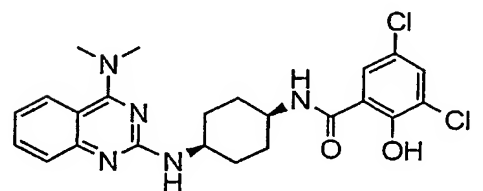
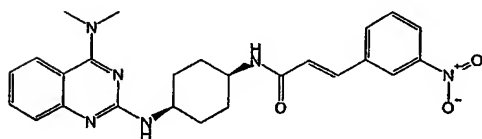
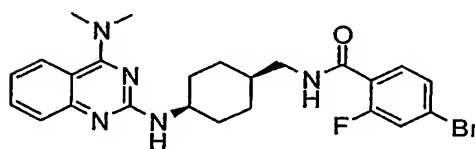
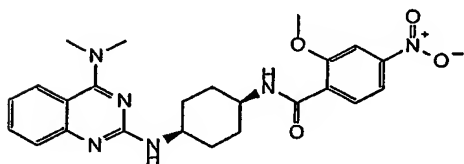
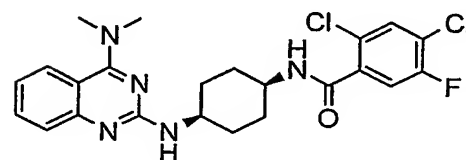
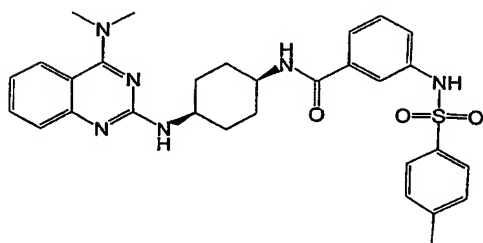
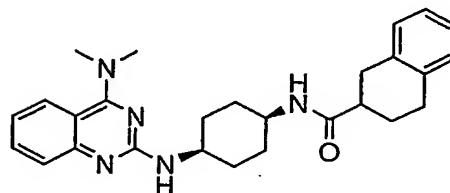
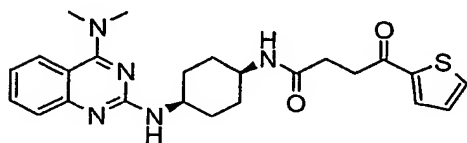
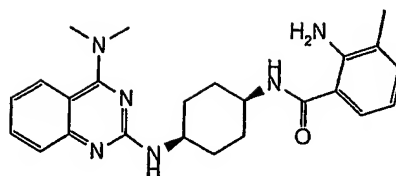
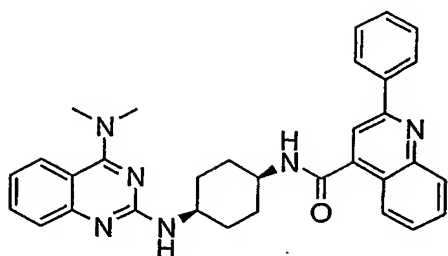


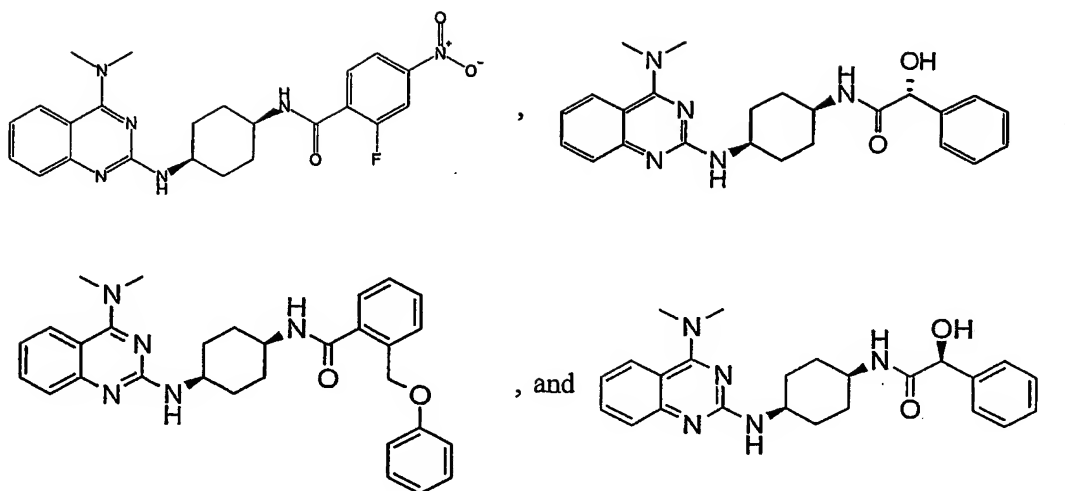












; or, in case of, a salt thereof.

7. A compound according to claim 3, wherein

R₁ represents

(i) C₁-C₁₀ alkyl,

C₁-C₁₀ alkyl substituted by substituent(s) independently selected from

•C₅-C₆ cycloalkyl,

•carbocyclic aryl,

•heterocyclyl,

(ii) C₃-C₆ cycloalkyl,

(iii) carbocyclic aryl,

(iv) or heterocyclyl;

L is selected from Formula XX - XXII;

wherein carbocyclic aryl is phenyl, naphthyl, anthranyl, or biphenyl;

heterocyclyl is 1,3-dioxo-isindolyl, 1*H*-indolyl, 1-oxo-3*H*-isobenzofuranyl, 2,3-dihydro-benzo[1,4]dioxinyl, 3,4-dihydro-2*H*-benzo[b][1,4]dioxepinyl, 4-oxo-3,4-dihydro-phthalazinyl, 9,10,10-trioxo-thioxanthenyl, 9*H*-xanthenyl, benzimidazolyl, benzo[1,3]dioxolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, furyl, imidazolyl, isoxazolyl, morpholino, oxolanyl, piperidyl, pyridyl, quinoxalyl, thienyl, quinolyl, or benzothiazolyl; or a salt thereof.

8. A compound according to claim 7, wherein

R₁ represents

(i) C₁-C₄ alkyl,

C₁-C₄ alkyl substituted by substituent(s) independently selected from

•cyclopentyl,

•carbocyclic aryl,

•heterocyclyl,

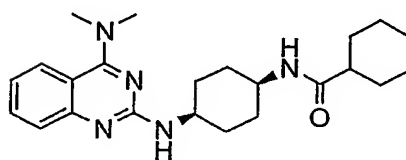
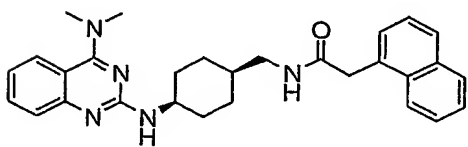
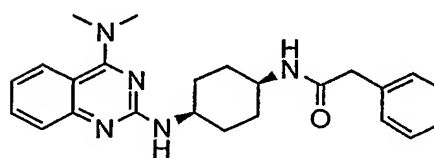
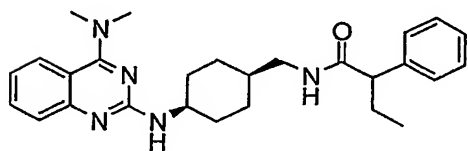
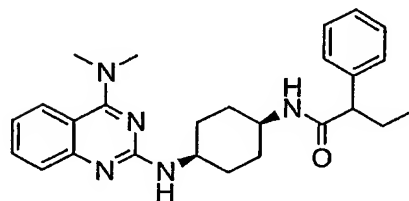
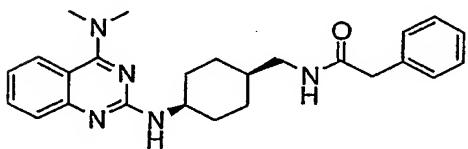
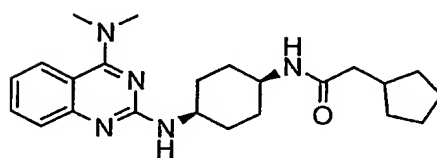
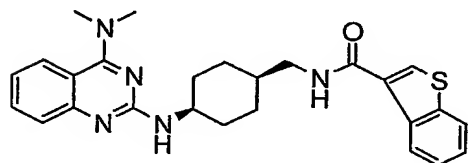
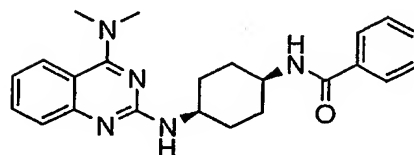
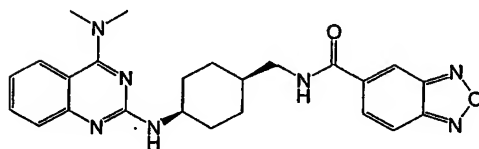
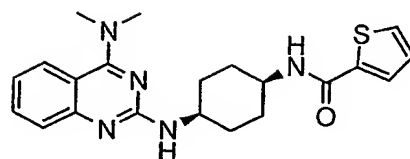
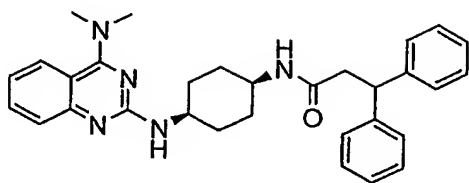
(ii) carbocyclic aryl,

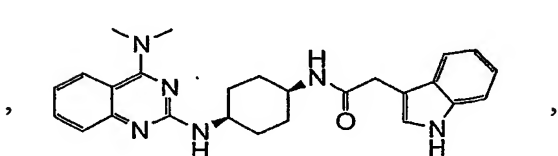
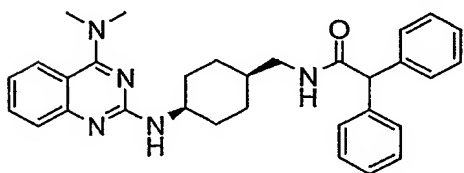
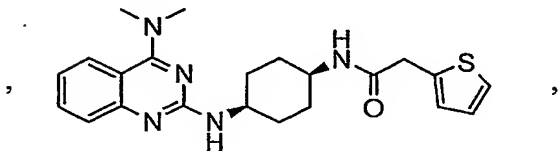
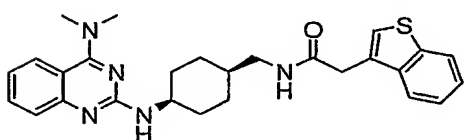
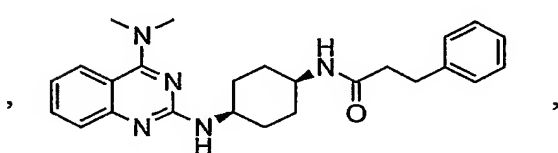
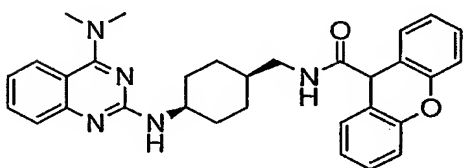
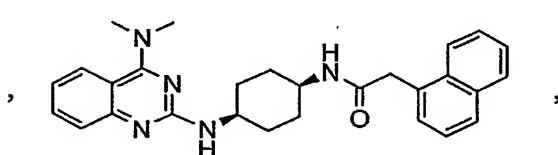
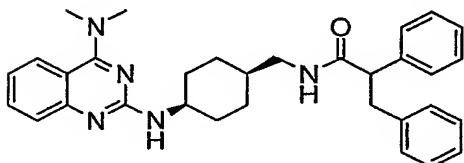
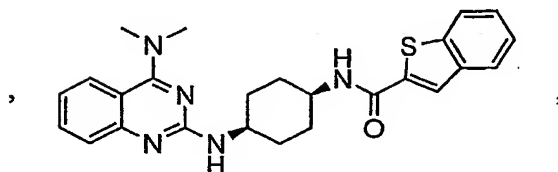
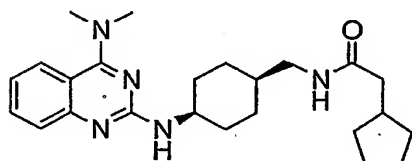
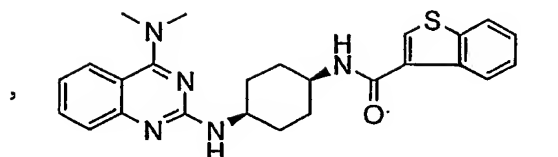
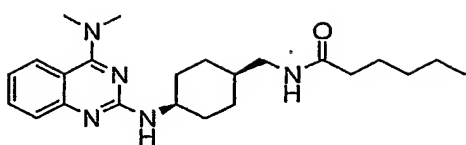
(iii) or heterocyclyl;

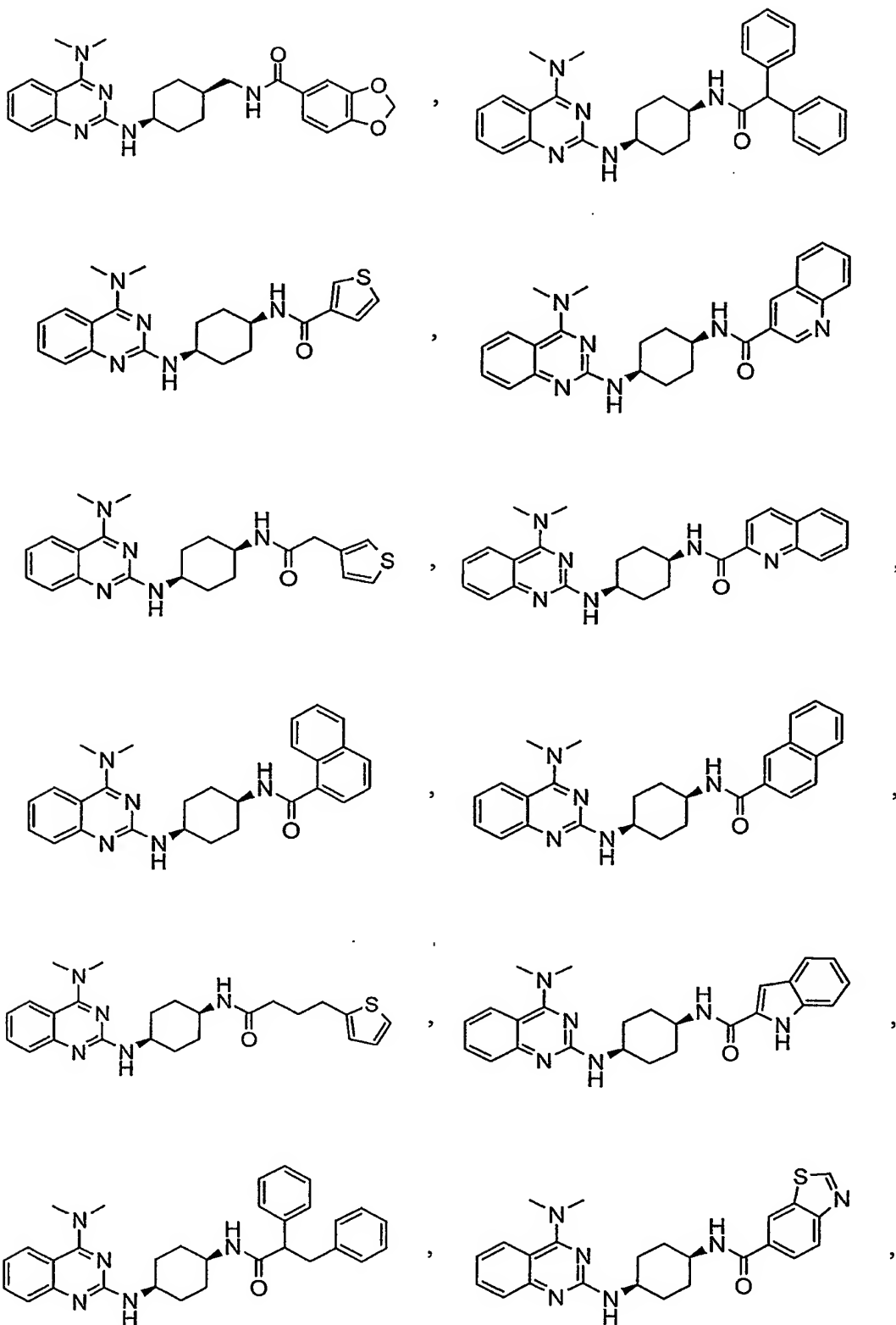
wherein carbocyclic aryl is phenyl, naphthyl, anthranyl, or biphenyl;

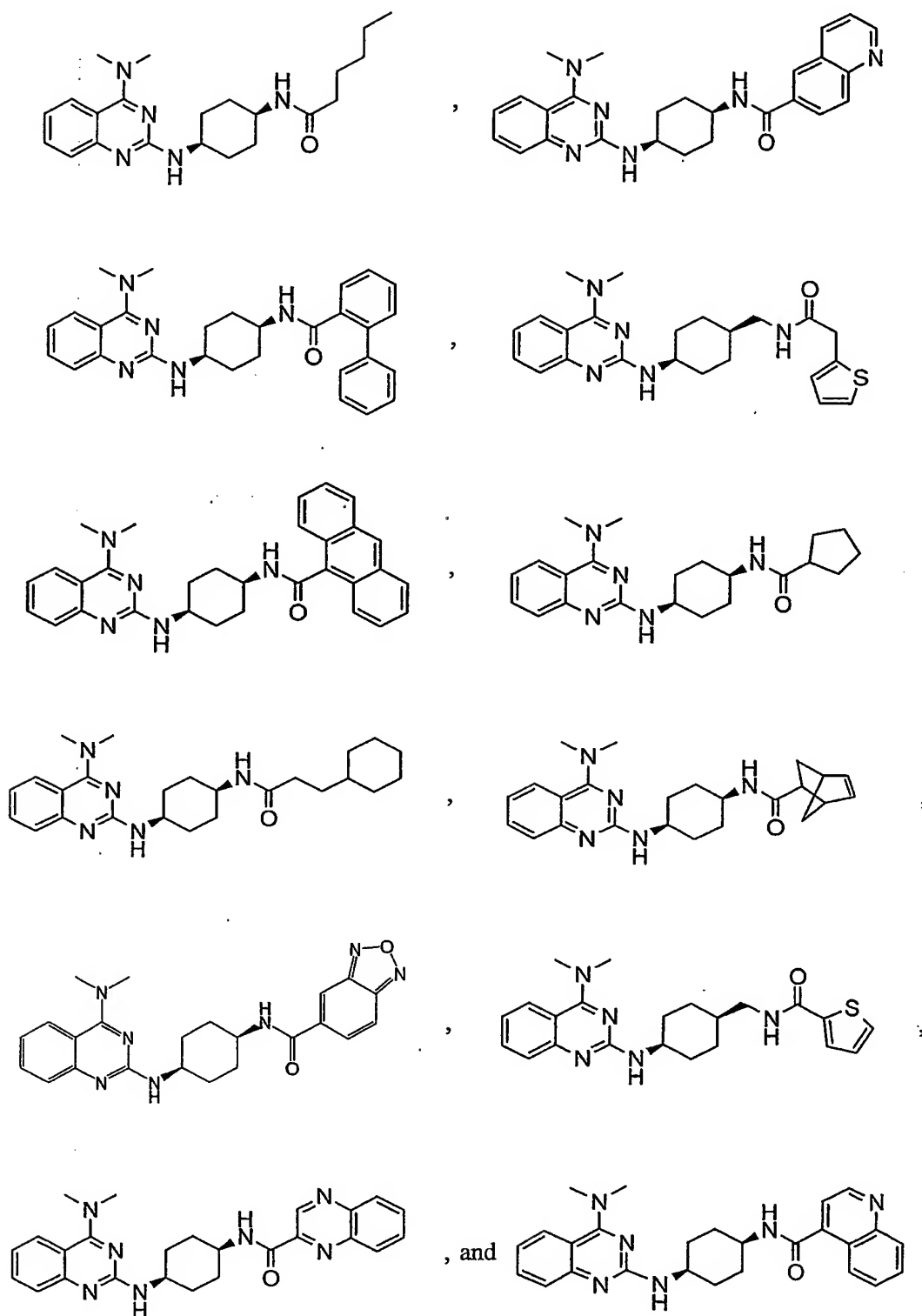
heterocyclyl is 9*H*-xanthenyl, benzo[1,3]dioxolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, thienyl, 1*H*-indolyl, quinoxalyl, quinolyl, or benzothiazolyl; or a salt thereof.

9. A compound according to claim 8 of Formula I thereof selected from the group consisting of









; or, in case of, a salt thereof.

10. A compound according to claim 1, wherein Q is Fomura II;

R₁ represents

- (i) C₁-C₁₀ alkyl,
- C₁-C₁₀ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - oxo,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy substituted by substituent(s) independently selected from
 - carbocyclic aryl,
 - heterocyclyl,
 - heterocyclyl substituted by C₁-C₃ alkyl,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by C₁-C₃ alkoxy,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - mono- or di-C₁-C₃ alkylamino,
 - mono- or di-C₁-C₃ alkylamino substituted by carbocyclic aryl,
 - mono- or di-C₁-C₃ alkylamino substituted by halogenated carbocyclic aryl,
 - mono- or di-C₁-C₃ alkylamino,
 - mono- or di-C₁-C₃ alkylamino substituted by substituent(s) independently selected from
 - cyano,
 - carbocyclic aryl,
 - heterocyclyl,
 - mono- or di-carbocyclic arylamino,
 - mono- or di-carbocyclic arylamino substituted by C₁-C₃ alkyl,
 - C₁-C₃ alkylcarbonylamino,
 - C₁-C₄ alkoxycarbonylamino,

- carbocyclic arylsulfonylamino,
- carbocyclic arylsulfonylamino substituted by substituent(s) independently selected from
 - nitro,
 - C₁-C₃ alkyl,
 - mono- or di-C₁-C₃ alkylamino,
 - C₁-C₃ alkylthio,
 - C₁-C₃ alkylthio substituted by substituent(s) independently selected from
 - mono- or di-carbocyclic arylamino,
 - halogenated mono- or di-carbocyclic arylamino,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkoxy,
 - carbocyclic arylthio,
 - carbocyclic arylthio substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - carbocyclic arylsulfonyl,
 - halogenated carbocyclic arylsulfonyl,
 - heterocyclylthio,
 - C₃-C₆ cycloalkyl,
 - C₃-C₆ cycloalkyl substituted by C₁-C₃ alkyl,
 - carbocyclyl,
 - carbocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - C₂-C₃ alkenyl,
 - C₂-C₃ alkenyl substituted by carbocyclic aryl,
 - C₂-C₃ alkenyl substituted by carbocyclic aryl substituted C₁-C₃ alkylsulfinyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,

- hydroxy,
- nitro,
- C₁-C₄ alkyl,
- C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - carbocyclic aryl,
 - mono- or di-carbocyclic arylamino,
 - mono- or di-carbocyclic arylamino substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
 - halogenated C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy substituted by substituent(s) independently selected from
 - halogen,
 - carbocyclic aryl,
 - carbocyclic aryloxy,
 - C₁-C₃ alkoxycarbonyl,
 - mono- or di-C₁-C₃ alkylamino,
 - C₁-C₃ alkylthio,
 - halogenated C₁-C₃ alkylthio,
 - C₁-C₃ alkylsulfonyl,
 - C₃-C₆ cycloalkyl,
 - carbocyclic aryl,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,

- C₁-C₃ alkoxy substituted by carbocyclic aryl,
- carbocyclic aryl,
- halogenated carbocyclic aryl,
- (ii) C₂-C₈ alkenyl,
C₂-C₈ alkenyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy substituted by carbocyclic aryl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - C₁-C₃ alkoxy,
 - halogenated C₁-C₃ alkoxy,
 - heterocyclyl,
 - heterocyclyl substituted by nitro,
- (iii) C₂-C₄ alkynyl,
C₂-C₄ alkynyl substituted by carbocyclic aryl,
- (iv) C₃-C₆ cycloalkyl,
C₃-C₆ cycloalkyl substituted by substituent(s) independently selected from
 - C₁-C₃ alkyl,
 - C₁-C₃ alkyl substituted by substituent(s) independently selected from
 - hydroxy,
 - oxo,
 - carbocyclic aryl,
 - mono- or di-C₁-C₃ alkylamino,
 - mono- or di-C₁-C₃ alkylamino substituted by carbocyclic aryl,
 - carbocyclic aryl,
- (v) C₃-C₆ cycloalkenyl,
C₃-C₆ cycloalkenyl substituted by C₁-C₃ alkyl,
- (vi) carbocyclyl,
carbocyclyl substituted by substituent(s) independently selected from

- hydroxy,
- nitro,
- (vii) carbocyclic aryl,
carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - nitro,
 - C₁-C₉ alkyl,
 - C₁-C₉ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - oxo,
 - C₁-C₃ alkoxy,
 - carbocyclic aryloxy,
 - mono- or di-C₁-C₃ alkylamino-N-oxy,
 - mono- or di-C₁-C₃ alkylamino,
 - mono- or di-C₁-C₃ alkylamino substituted by carbocyclic aryl,
 - mono- or di-carbocyclic arylamino,
 - mono- or di-carbocyclic arylamino substituted by C₁-C₃ alkoxy,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - heterocyclyl,
 - heterocyclyl substituted by C₁-C₃ alkyl,
 - C₂-C₃ alkenyl,
 - C₂-C₃ alkenyl substituted by carbocyclic aryl,
 - C₁-C₉ alkoxy,
 - C₁-C₉ alkoxy substituted by substituent(s) independently selected from
 - hydroxy,
 - halogen,
 - carboxy,
 - mono- or di-C₁-C₃ alkylamino,

- carbocyclic aryl,
- halogenated carbocyclic aryl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl,
 - C₂-C₃ alkenyloxy,
 - C₁-C₃ alkylcarbonyloxy,
- carbocyclic aryloxy,
- carbocyclic aryloxy substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₄ alkyl,
 - halogenated C₁-C₄ alkyl,
 - C₁-C₃ alkoxy,
- heterocyclyloxy,
- heterocyclyloxy substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl,
- (carbocyclic aryl)S(O)₂O,
- carboxy,
- C₁-C₃ alkoxy carbonyl,
- mono- or di-C₁-C₃ alkylaminocarbonyl,
- mono- or di-C₁-C₃ alkylaminocarbonyl substituted by carbocyclic aryl,
- amino,
- mono- or di-C₁-C₄ alkylamino,
- mono- or di-C₁-C₄ alkylamino substituted by cyano,
- mono- or di-carbocyclic arylamino,
- C₁-C₃ alkylcarbonylamino,

- carbocyclic arylsulfonylamino,
- carbocyclic arylsulfonylamino substituted by C₁-C₃ alkyl,
- (carbocyclic aryl)NHC(O)NH,
- (carbocyclic aryl)NHC(O)NH substituted by C₁-C₃ alkoxy,
- (carbocyclic aryl)NHC(O)NH substituted by halogenated C₁-C₃ alkoxy,
- C₁-C₃ alkylthio,
- halogenated C₁-C₃ alkylthio,
- carbocyclic arylthio,
- halogenated carbocyclic arylthio,
- carbocyclic arylthio substituted by C₁-C₃ alkyl,
- heterocyclylthio,
- C₁-C₃ alkylsulfonyl,
- mono- or di-C₁-C₃ alkylaminosulfonyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - C₁-C₇ alkyl,
 - halogenated C₁-C₇ alkyl,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - C₁-C₃ alkyl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
- (viii) heterocyclyl,
- or heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,

- oxo,
- C₁-C₃ alkylcarbonyloxy,
- C₁-C₃ alkoxycarbonyl,
- C₁-C₃ alkylthio,
- C₁-C₃ alkylthio substituted by carbocyclic aryl,
- C₁-C₃ alkylthio substituted by halogenated carbocyclic aryl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - heterocyclyl,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy substituted by carbocyclic aryl,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by C₁-C₃ alkyl,
 - mono- or di-C₁-C₃ alkylamino,
 - C₁-C₄ alkylcarbonylamino,
 - C₁-C₃ alkylthio,
 - carbocyclic arylthio,
 - halogenated carbocyclic arylthio,
 - carbocyclic arylthio substituted by C₁-C₃ alkoxycarbonyl,
 - heterocyclylthio,
 - heterocyclylthio substituted by C₁-C₃ alkyl,
 - C₁-C₃ alkylsulfonyl,
 - carbocyclic arylsulfonyl,
 - carbocyclic arylsulfonyl substituted by C₁-C₄ alkyl,
 - C₁-C₃ alkoxycarbonyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₃ alkyl,

- halogenated C₁-C₃ alkyl,
- C₁-C₃ alkoxy,
- halogenated C₁-C₃ alkoxy,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
- C₁-C₃ alkyl,
- halogenated C₁-C₃ alkyl,
- C₁-C₃ alkoxy,
- C₁-C₃ alkoxycarbonyl;

Y is -(CH₂)_m, m is 0 or 1;

wherein carbocyclic aryl is phenyl, naphthyl, biphenyl, or phenanthryl;
 carbocyclyl is 9*H*-fluorenyl, 9-oxo-fluorenyl, acenaphthyl, anthraquinonyl, indanyl, or indenyl;

heterocyclyl is 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1,3,4-thiadiazolyl, 1,3-dioxo-isoindolyl, 1,3-dioxolanyl, 1*H*-indolyl, 1*H*-pyrrolo[2,3-*c*]pyridyl, 1*H*-pyrrolyl, 2,2',5',2''-terthiophenyl, 2,2'-bithiophenyl, 2,3-dihydro-1-oxo-isoindolyl, 2,3-dihydro-benzo[1,4]dioxinyl, 2,3-dihydro-benzofuryl, 2,4-dihydro-3-oxo-pyrazolyl, 2*H*-benzopyranyl, 2-oxo-pyrrolidinyl, 3,4-dihydro-2*H*-benzo[1,4]oxazinyl, 3,4-dihydro-2*H*-benzo[*b*][1,4]dioxepinyl, 4*H*-benzo[1,3]dioxinyl, 4*H*-benzopyranyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, 4-oxo-benzopyranyl, 9*H*-carbazolyl, 9*H*-xanthenyl, azetidiny, benzimidazolyl, benzo[1,3]dioxolyl, benzo[*b*]thienyl, benzofuryl, benzothiazolyl, furyl, imidazo[2,1-*b*]thiazolyl, imidazolyl, isoxazolyl, morpholino, morpholinyl, oxolanyl, piperazyl, piperidyl, pyrazolo[5,1-*b*]thiazolyl, pyrazolyl, pyridyl, pyrimidyl, pyrrolidyl, quinolyl, quinoxalyl, thiazolidyl, thiazolyl, thienyl, or thiolanyl;

halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

11. A compound according to claim 10, wherein

R₁ represents

- (i) C₁-C₁₀ alkyl substituted by substituent(s) independently selected from
- methoxy,
- methoxy substituted by carbocyclic aryl,

- carbocyclic aryloxy,
- halogenated carbocyclic aryloxy,
- mono-C₁-C₂ alkylamino substituted by cyano,
- mono- or di-C₁-C₂ alkylamino substituted by carbocyclic aryl,
- mono-carbocyclic arylamino,
- mono-carbocyclic arylamino substituted by methyl,
- carbocyclic arylsulfonylamino substituted by methyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by carbocyclic aryl,
 - C₁-C₄ alkyl substituted by hydroxy,
 - C₁-C₂ alkoxy,
 - halogenated C₁-C₂ alkoxy,
 - heterocyclyl substituted by carbocyclic aryl,
- (ii) C₂-C₈ alkenyl substituted by substituent(s) independently selected from
 - methoxy substituted by carbocyclic aryl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by methoxy,
- (iii) C₂-C₄ alkynyl substituted by carbocyclic aryl,
- (iv) cyclohexyl substituted by carbocyclic arylmethyl,
- (v) carbocyclyl,
- (vi) carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - amino,
 - C₁-C₉ alkyl,
 - halogenated C₁-C₉ alkyl,

- C₁-C₉ alkoxy,
- C₁-C₉ alkoxy substituted by substituent(s) independently selected from
 - halogen,
 - halogenated carbocyclic aryl,
 - propenyloxy,
 - methylamino,
 - di-C₁-C₂ alkylamino,
 - di-C₁-C₂ alkylamino substituted by cyano,
 - methylthio,
 - halogenated methylthio,
- (vii) heterocyclyl,
- or heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by hydroxy,
 - C₁-C₄ alkyl substituted by carbocyclic aryl,
 - methoxy,
 - C₁-C₂ alkoxycarbonyl,
 - carbocyclic arylthio substituted by methoxycarbonyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - halogenated methyl,
 - heterocyclyl;

R₂ is methylamino or dimethylamino;

L is selected from Formula Va, VIIIa, or IXa;

wherein carbocyclic aryl is phenyl, naphthyl, biphenyl, or phenanthryl;

carbocyclyl is 9*H*-fluorenyl, acenaphthyl, or anthraquinonyl;

heterocyclyl is 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1,3-dioxolanyl, 1*H*-indolyl, 1*H*-pyrrolyl, 2,2',5',2''-terthiophenyl, 2,2'-bithiophenyl, 2,3-dihydro-benzo[1,4]dioxinyl, 3,4-dihydro-2*H*-benzo[1,4]oxazinyl, 4-oxo-benzopyranyl, 9*H*-carbazolyl, 9*H*-xanthenyl, benzimidazolyl, benzo[1,3]dioxolyl, benzo[b]thienyl, benzofuryl,

benzothiazolyl, furyl, imidazolyl, isoxazolyl, oxolanyl, pyrazolo[5,1-b]thiazolyl, pyrazolyl, pyridyl, pyrimidyl, quinolyl, quinoxalyl, thiazolidyl, thiazolyl, thienyl, 2*H*-benzopyranyl, 4*H*-benzo[1,3]dioxinyl, azetidyl, imidazo[2,1-b]thiazolyl, morpholinyl, or 2,3-dihydro-benzofuryl;

halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

12. A compound according to claim 11, wherein

R₁ represents

(i) C₁-C₇ alkyl substituted by substituent(s) independently selected from

- methoxy,
- methoxy substituted by carbocyclic aryl,
- carbocyclic aryloxy,
- halogenated carbocyclic aryloxy,
- mono-ethylamino substituted by cyano,
- di-methylamino substituted by carbocyclic aryl,
- mono-carbocyclic arylamino,
- mono-carbocyclic arylamino substituted by methyl,
- carbocyclic arylsulfonylamino substituted by methyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by carbocyclic aryl,
 - C₁-C₄ alkyl substituted by hydroxy,
 - methoxy,
 - halogenated methoxy,
 - heterocyclyl substituted by carbocyclic aryl,

(ii) C₂-C₇ alkenyl substituted by substituent(s) independently selected from

- methoxy substituted by carbocyclic aryl,
- carbocyclic aryl,

- carbocyclic aryl substituted by methoxy,
- (iii) butynyl substituted by carbocyclic aryl,
- (iv) cyclohexyl substituted by carbocyclic arylmethyl,
- (v) carbocyclyl,
- (vi) carbocyclic aryl,
carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - amino,
 - C₁-C₂ alkyl,
 - halogenated methyl,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy substituted by substituent(s) independently selected from
 - halogen,
 - halogenated carbocyclic aryl,
 - propenyloxy,
 - di-C₁-C₂ alkylamino,
 - di-C₁-C₂ alkylamino substituted by cyano,
 - methylthio,
 - halogenated methylthio,
 - (vii) heterocyclyl,
or heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkyl substituted by hydroxy,
 - C₁-C₃ alkyl substituted by carbocyclic aryl,
 - methoxy,
 - ethoxycarbonyl,
 - carbocyclic arylthio substituted by methoxycarbonyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from

- halogen,
- halogenated methyl,
- heterocyclyl;

L is selected from Formula XX - XXII;

wherein carbocyclic aryl is phenyl, **naphthyl**, or biphenyl;

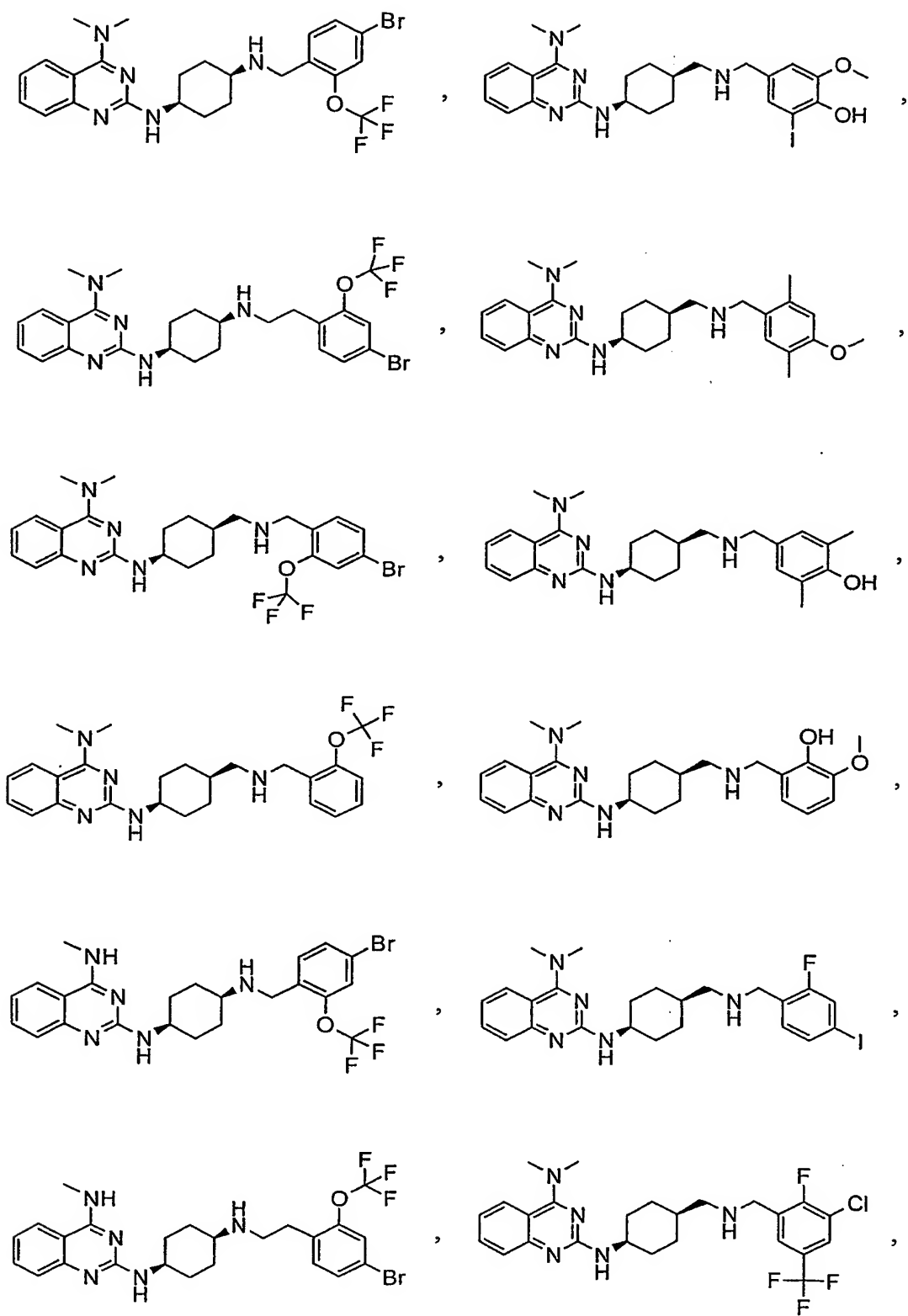
carbocyclyl is acenaphthyl;

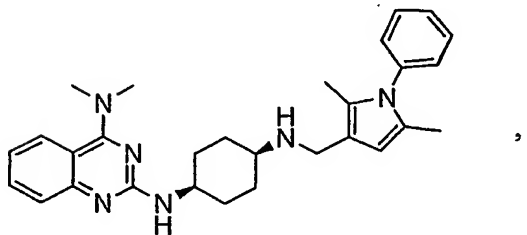
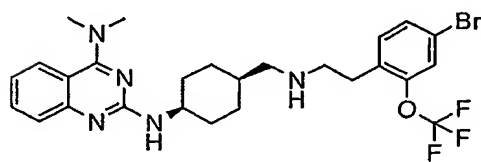
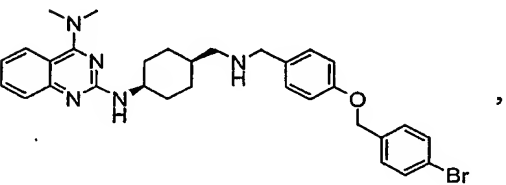
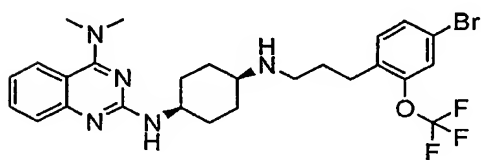
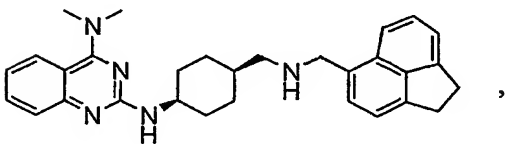
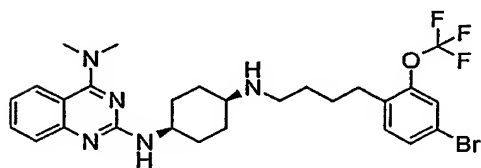
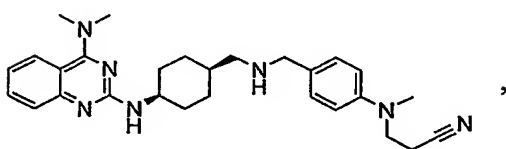
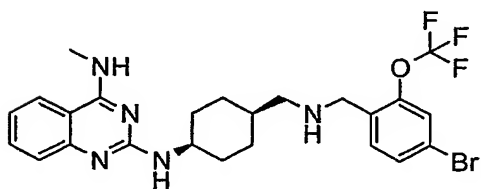
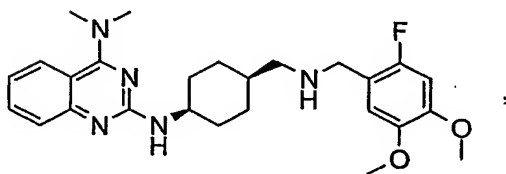
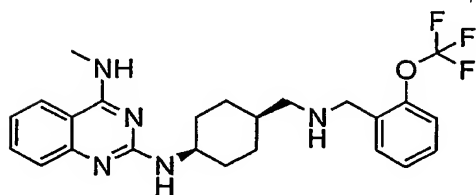
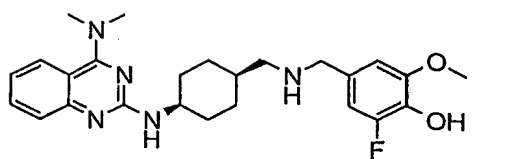
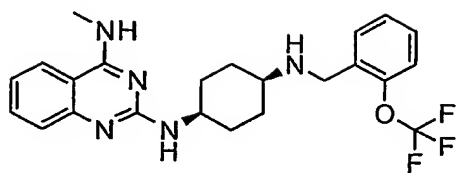
heterocyclyl is 1*H*-indolyl, 1*H*-pyrrolyl, 2,3-dihydro-benzo[1,4]dioxinyl, 9*H*-carbazolyl, benzo[1,3]dioxolyl, furyl, pyrazolyl, thienyl, 4-oxo-benzopyranyl, azetidiny, imidazo[2,1-*b*]thiazolyl, pyridyl, imidazolyl, 2,3-dihydro-benzofuryl, or benzo[*b*]thienyl;

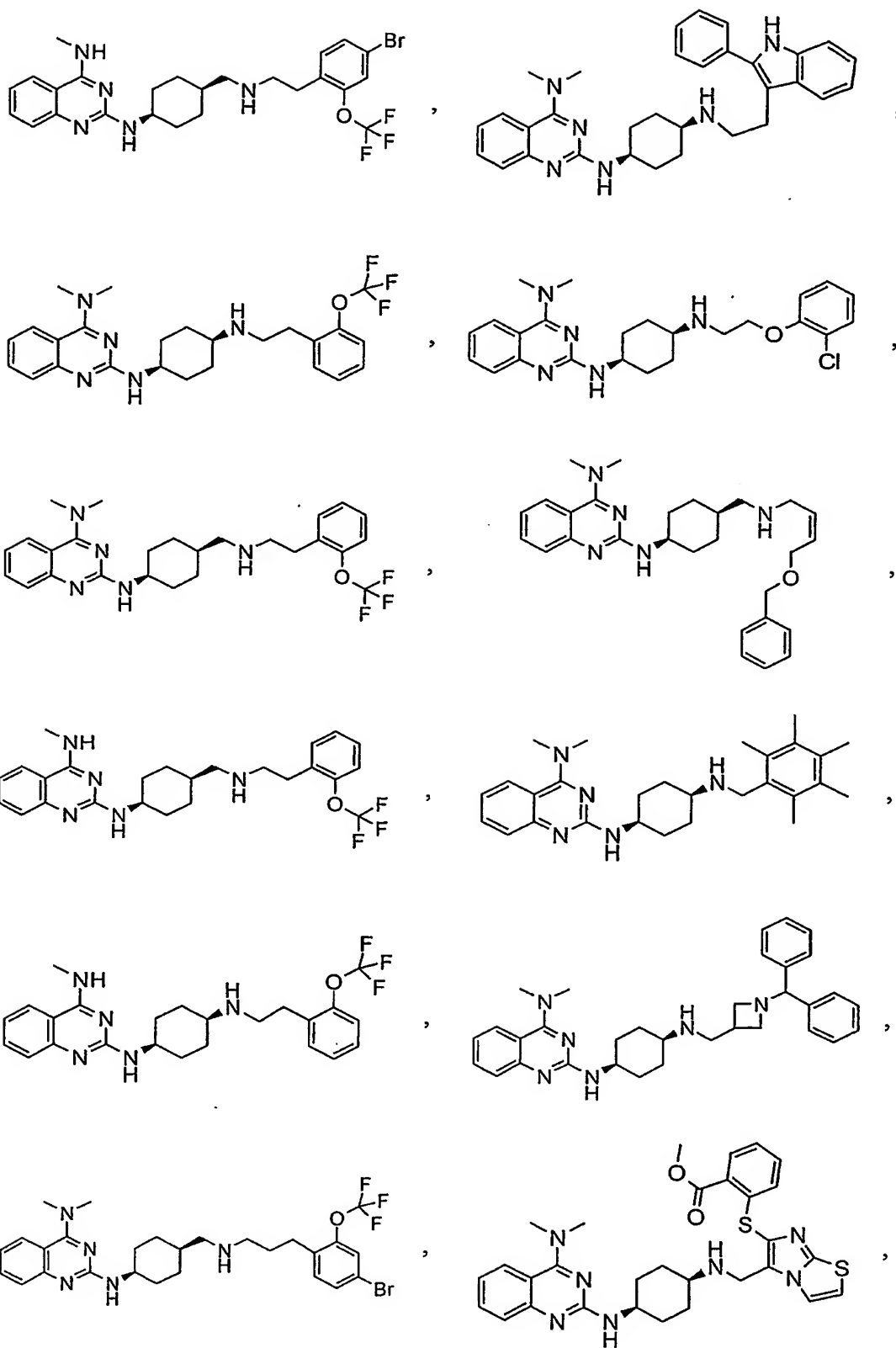
halogen is fluoro, chloro, bromo, or iodo;

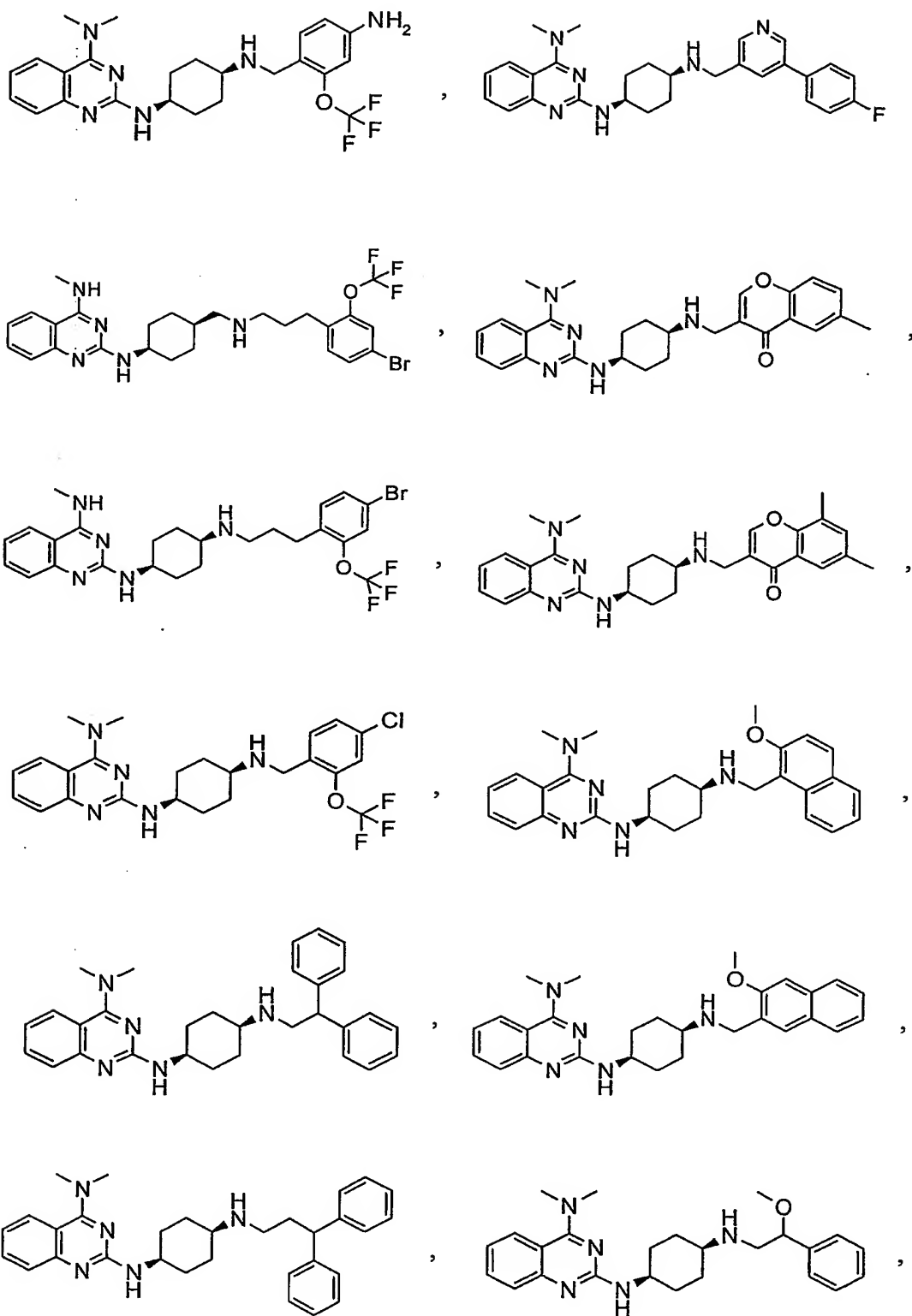
or a salt thereof.

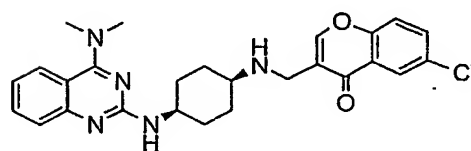
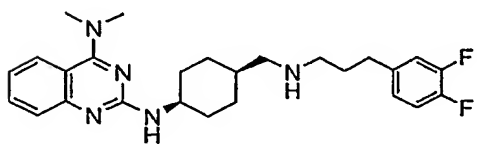
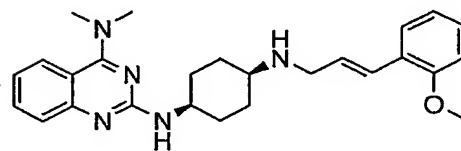
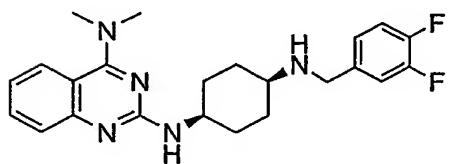
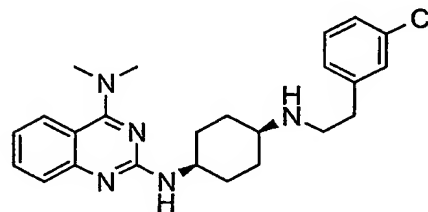
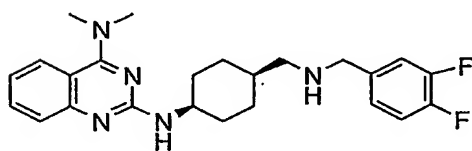
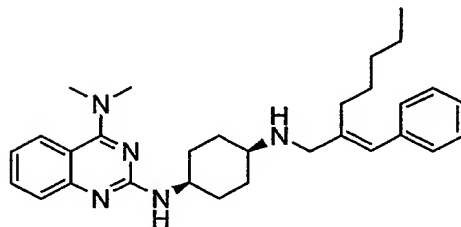
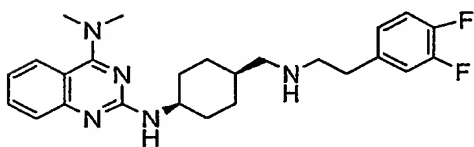
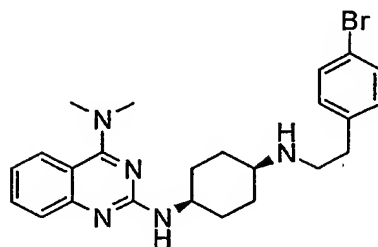
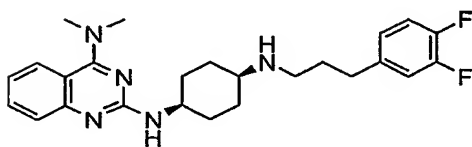
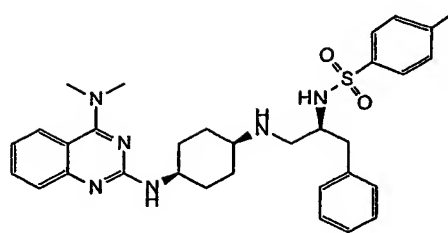
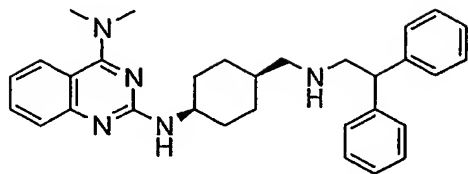
13. A compound according to claim 12 of Formua I selected from the group consisting of

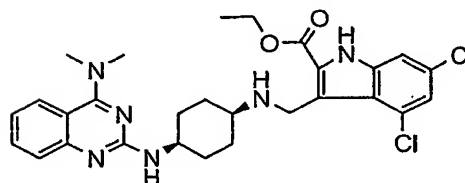
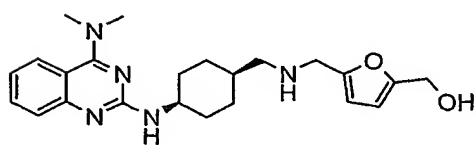
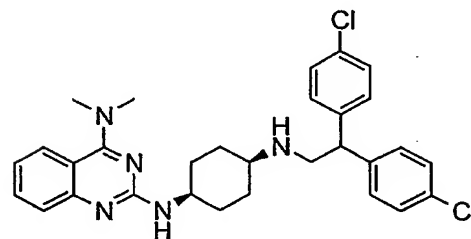
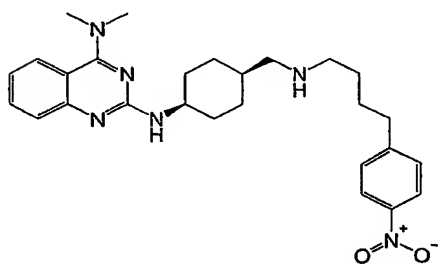
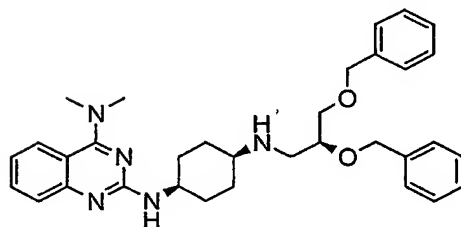
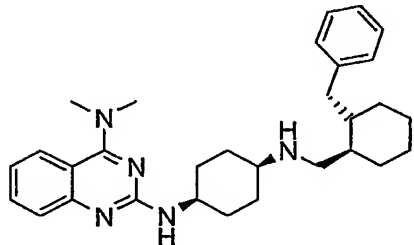
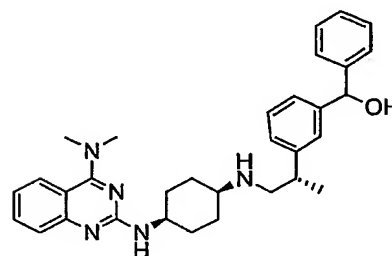
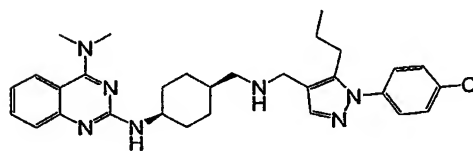
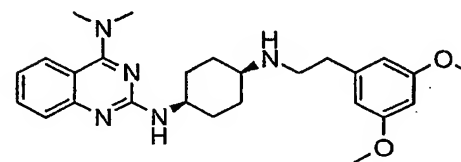
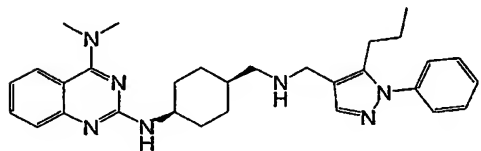
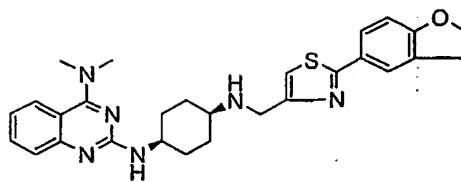
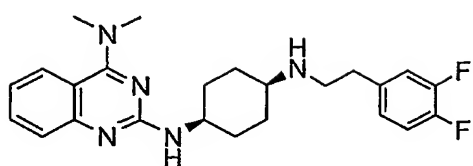


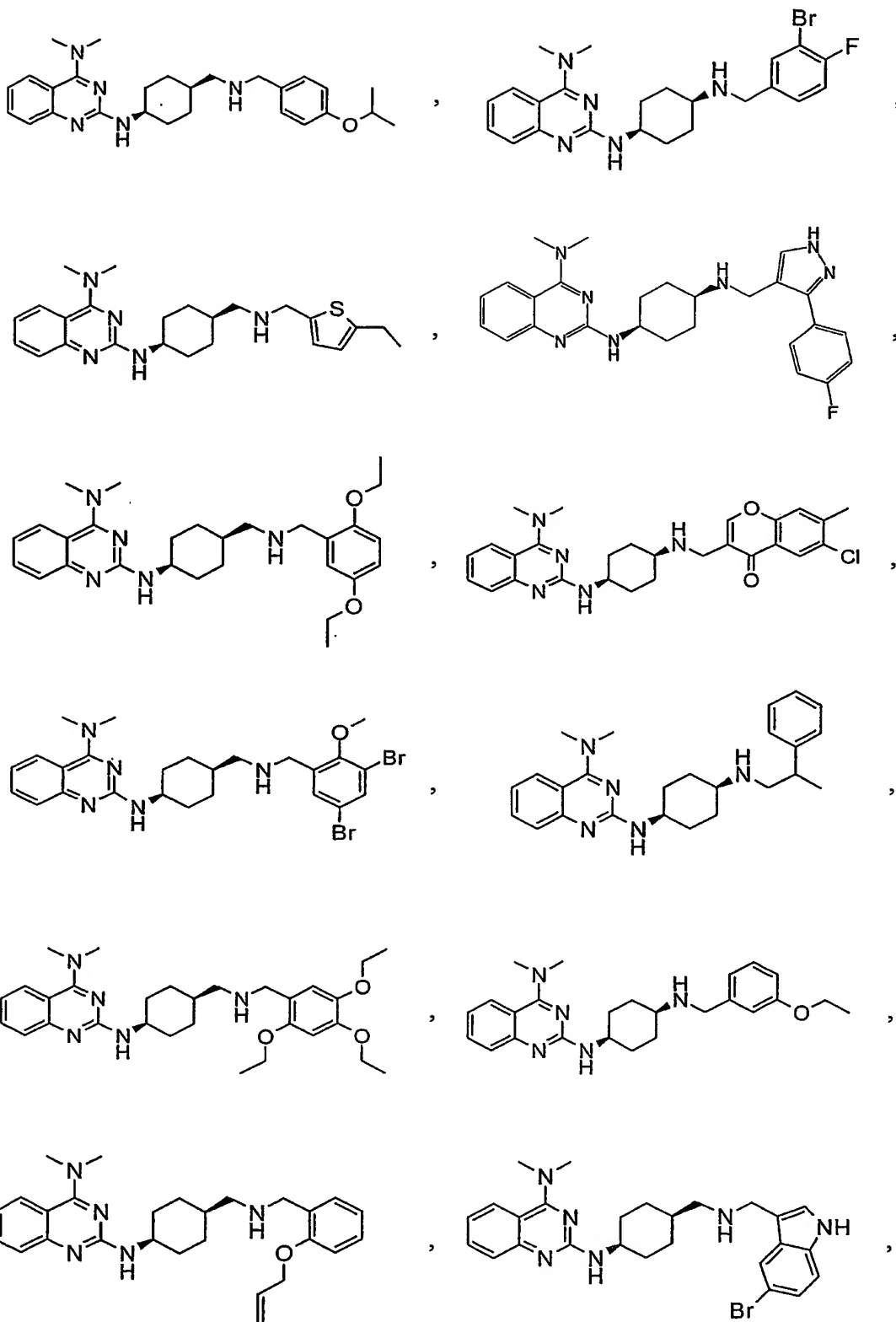


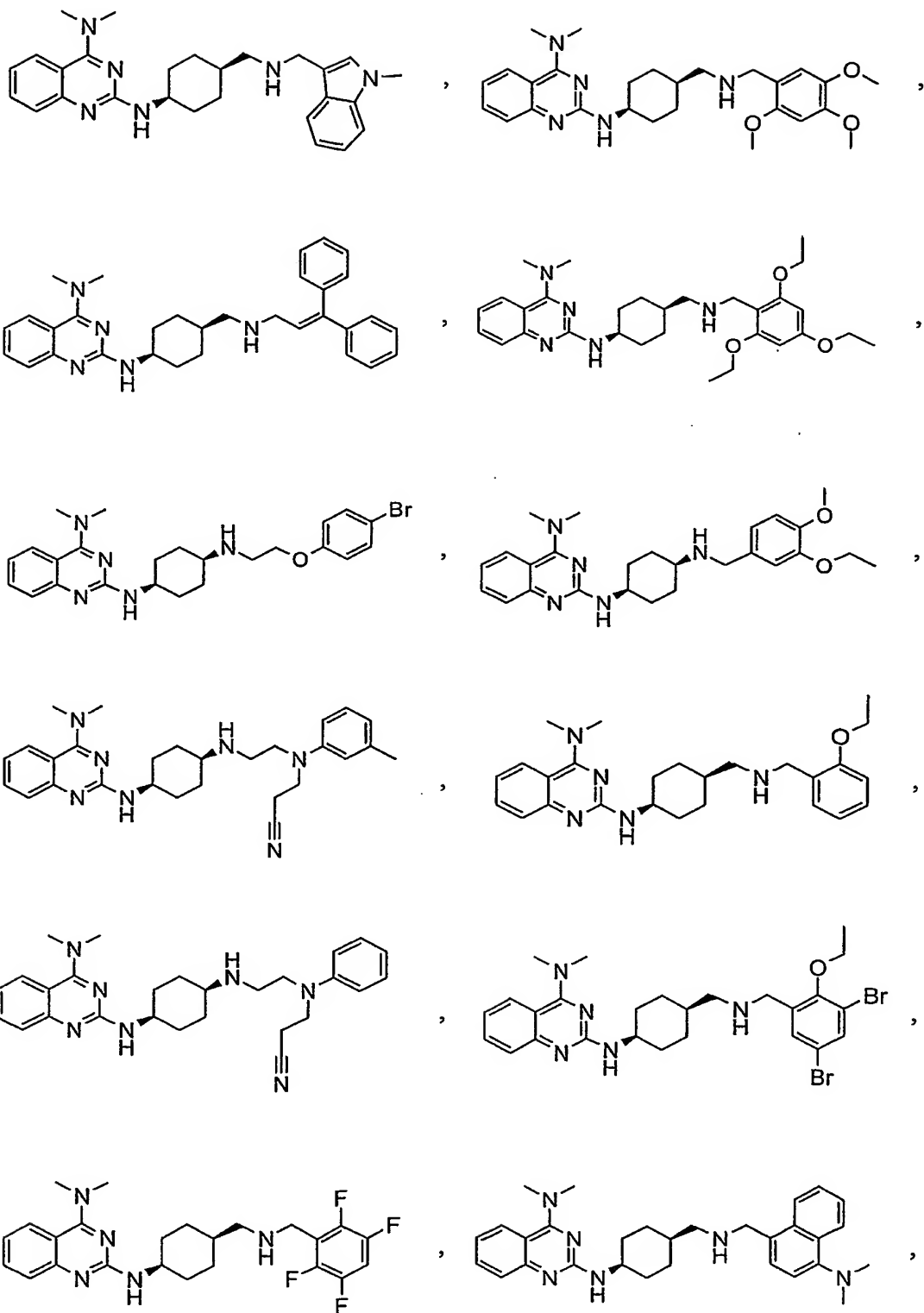


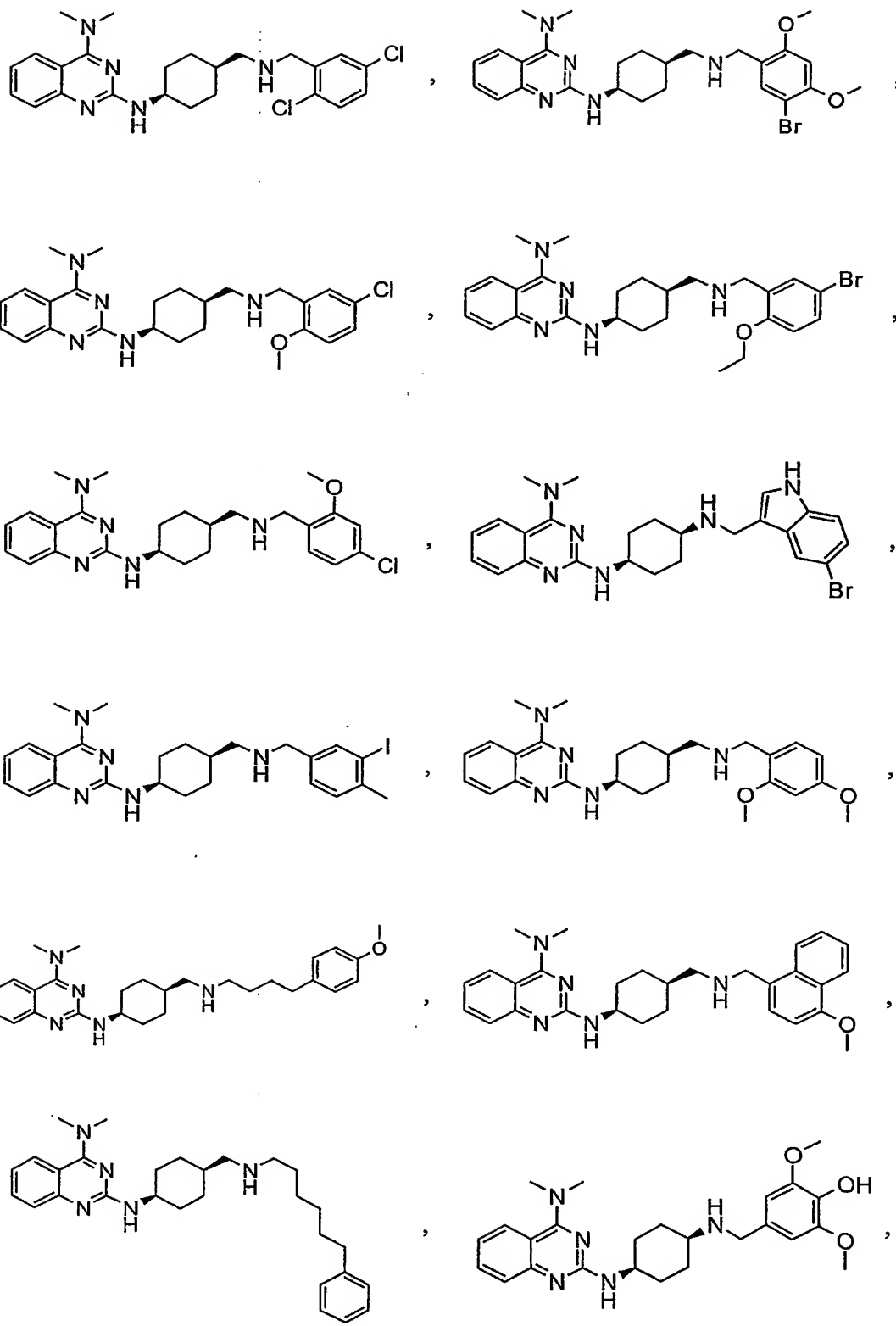


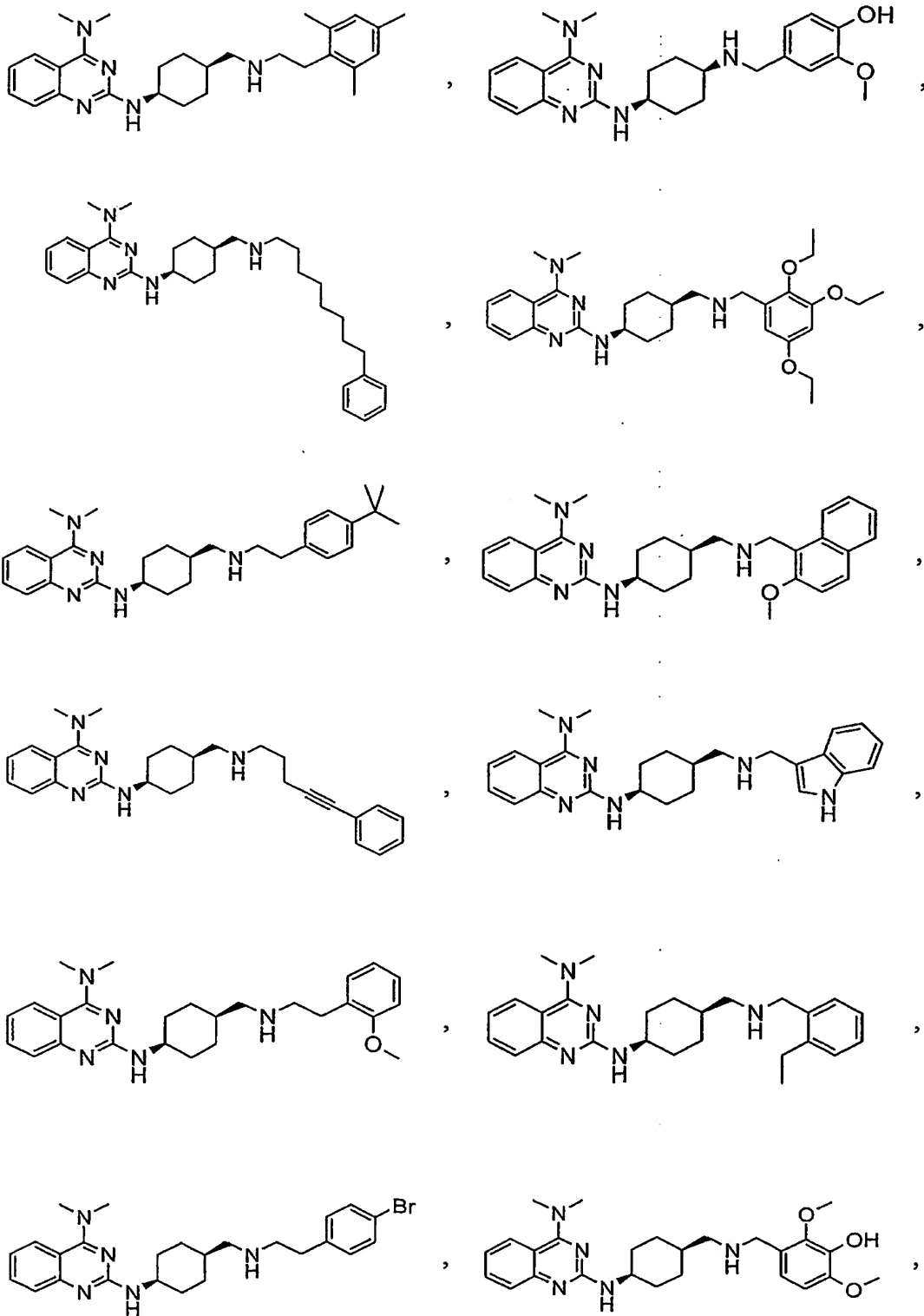


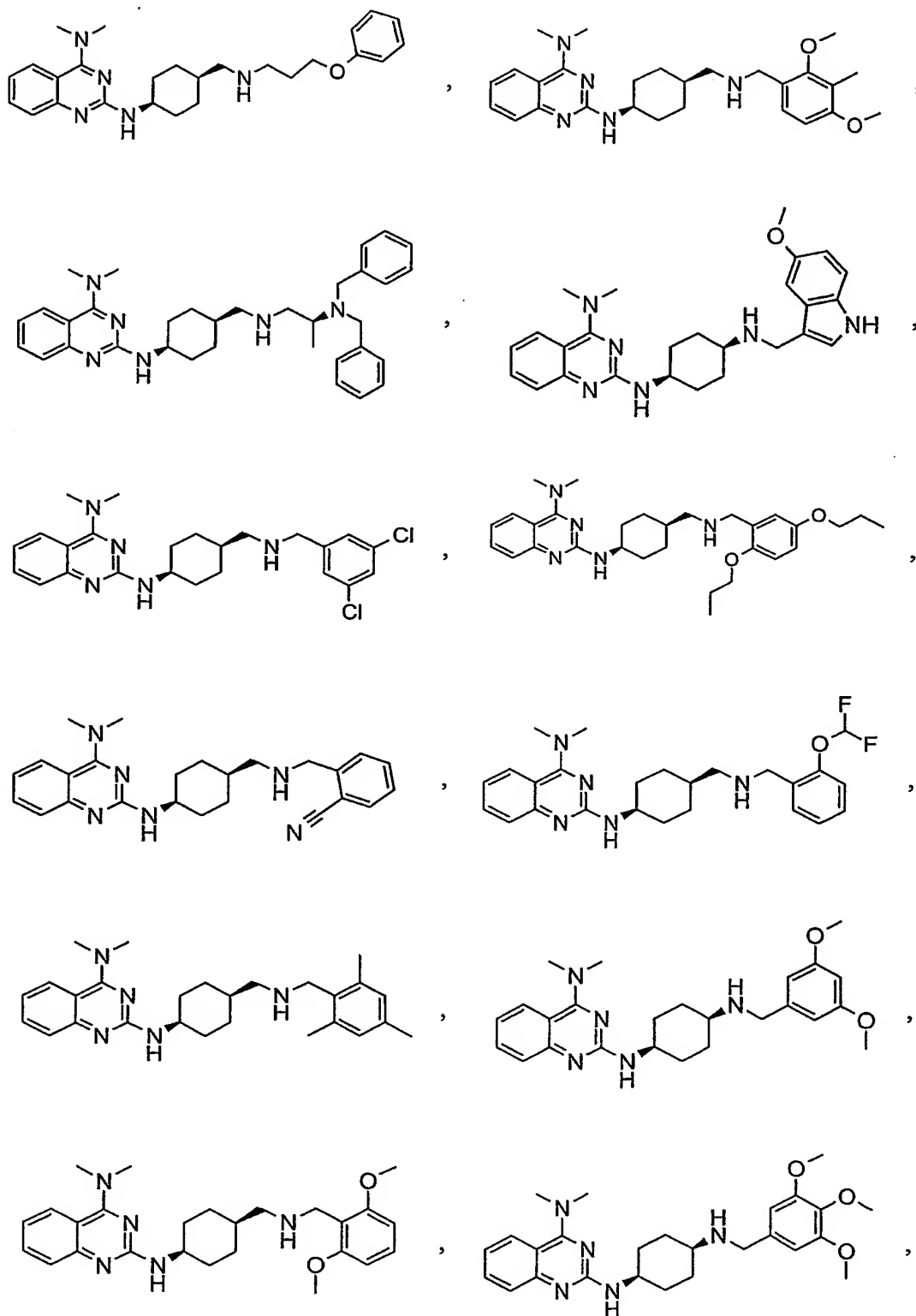


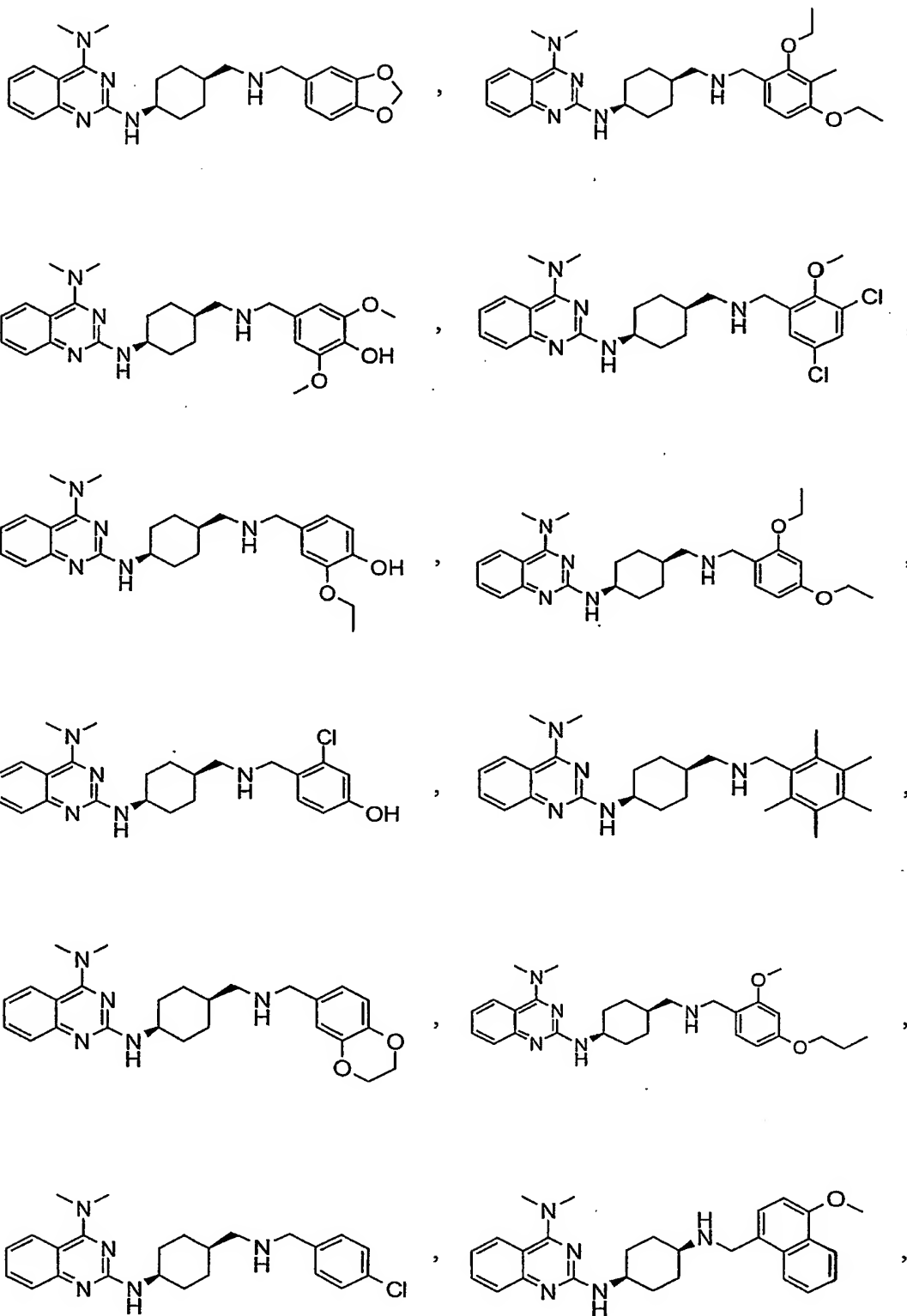


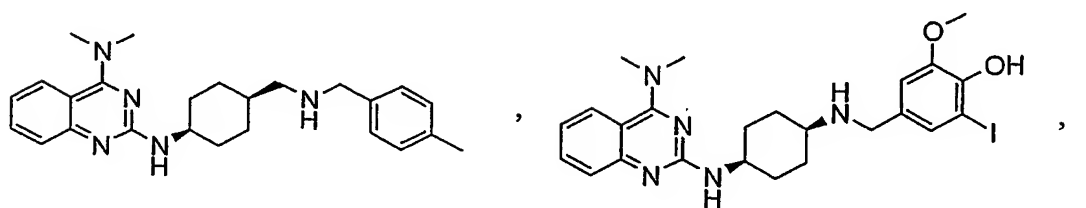
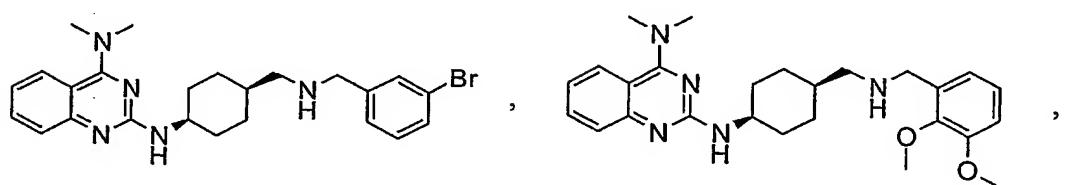
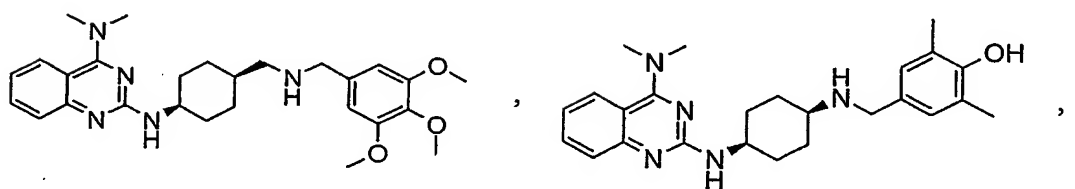
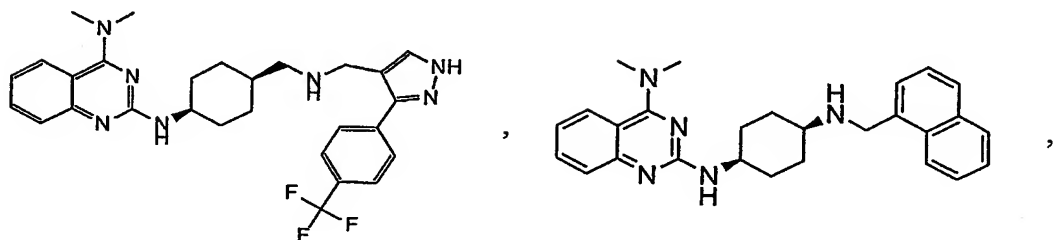
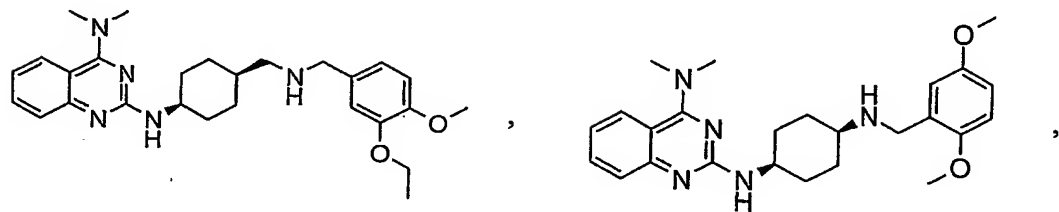
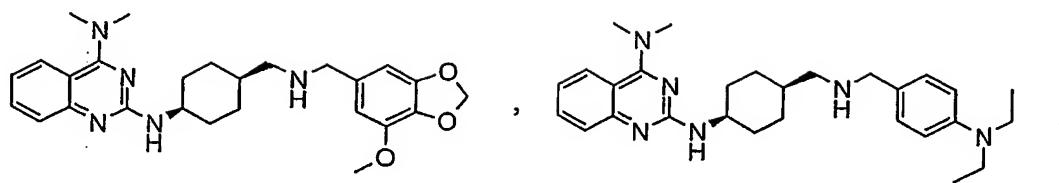


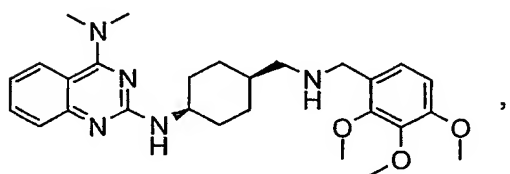
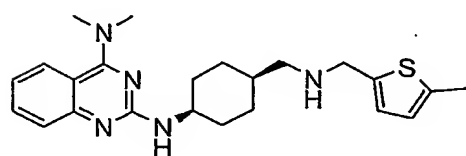
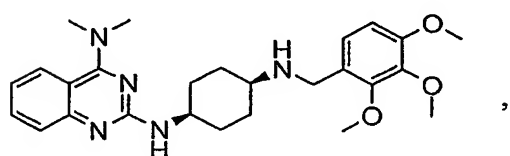
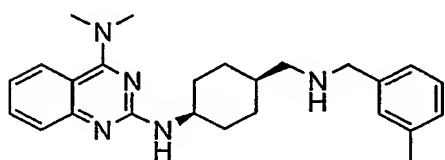
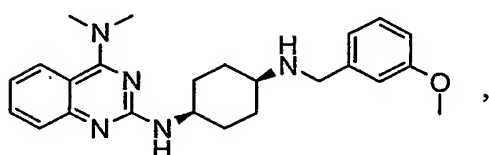
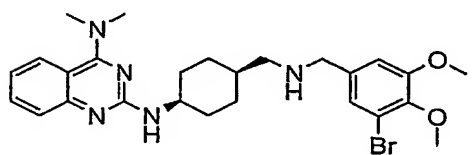
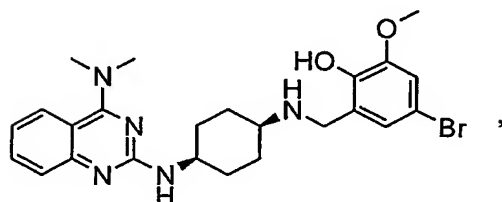
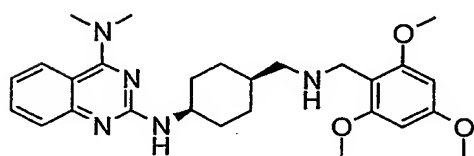
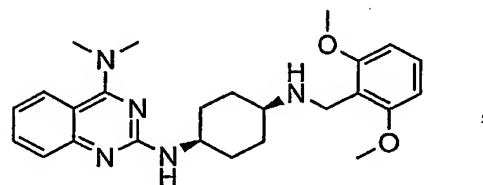
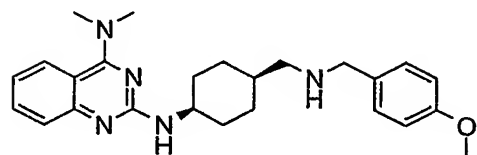
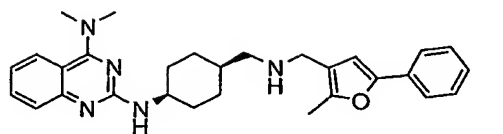
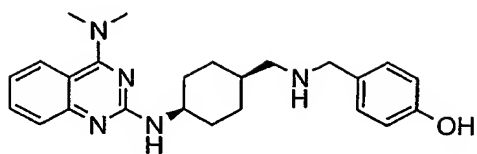


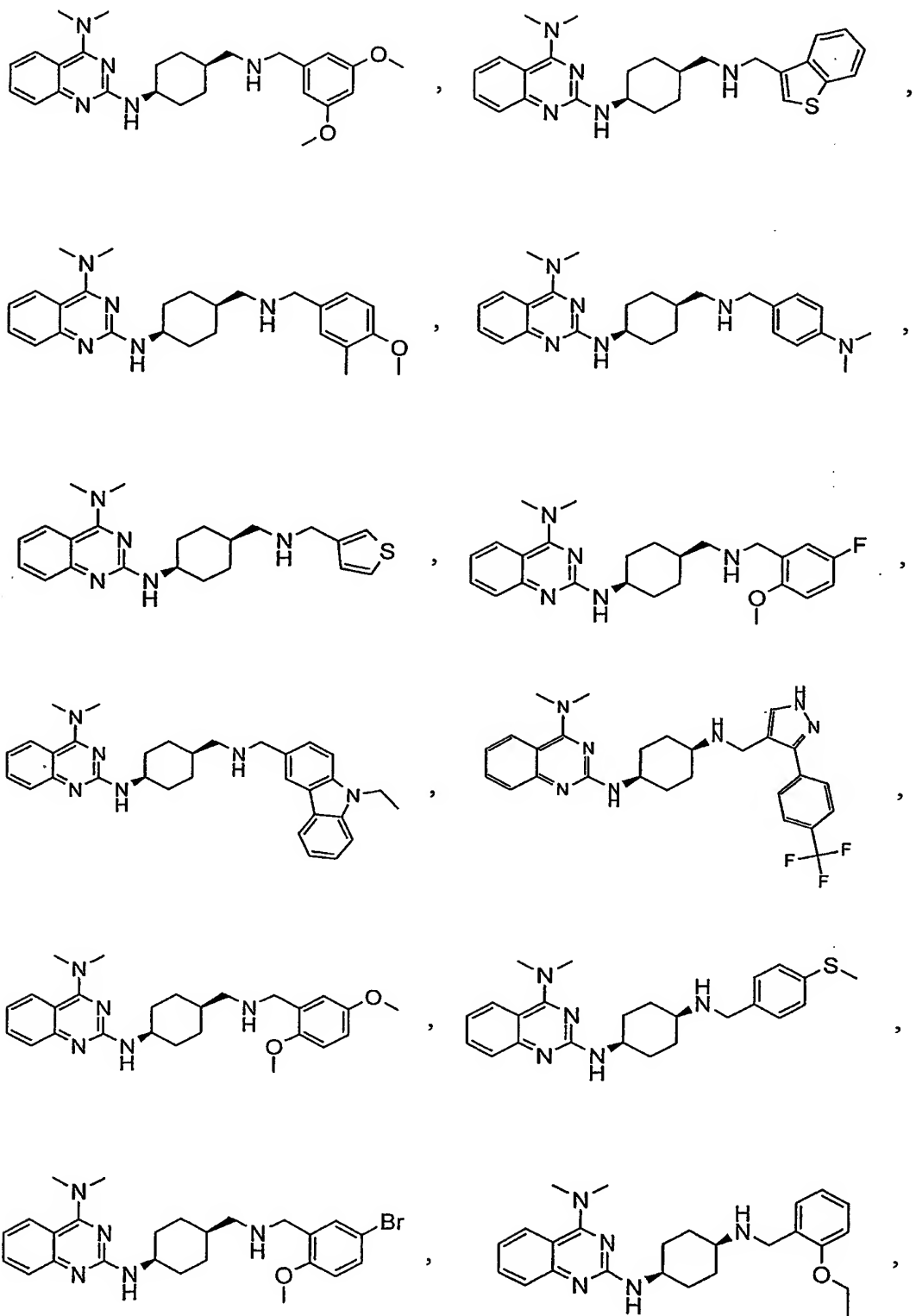


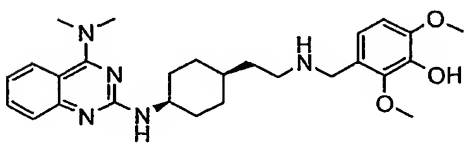
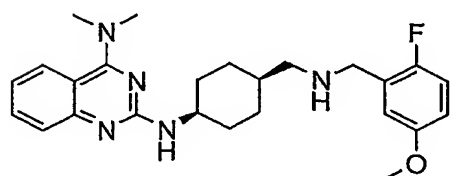
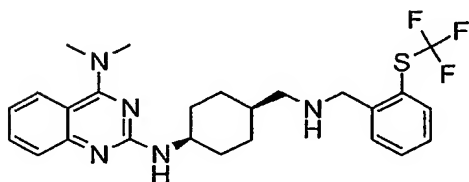
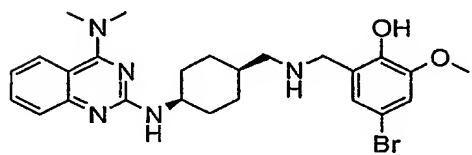
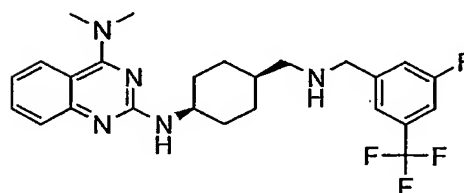
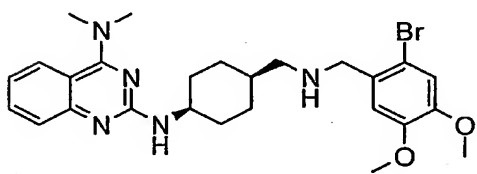
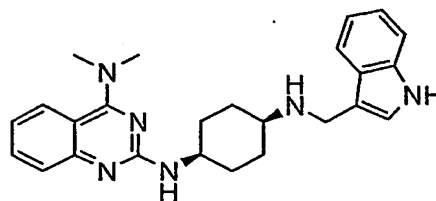
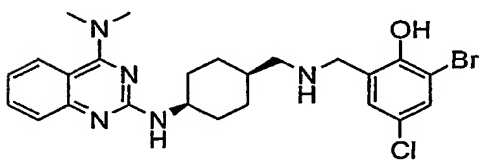
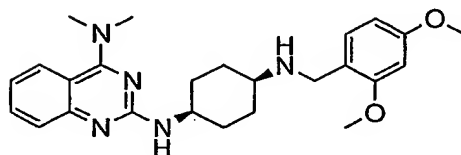
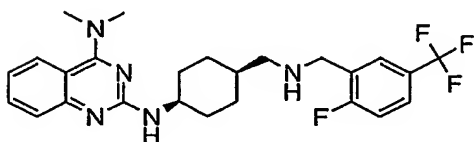
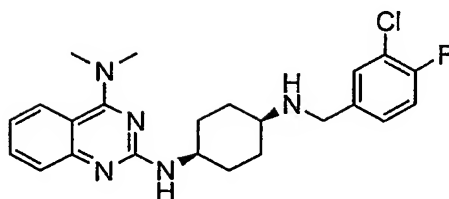
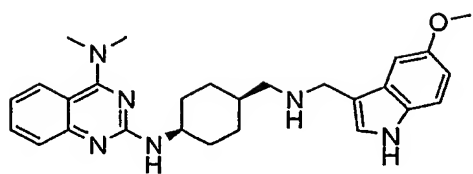


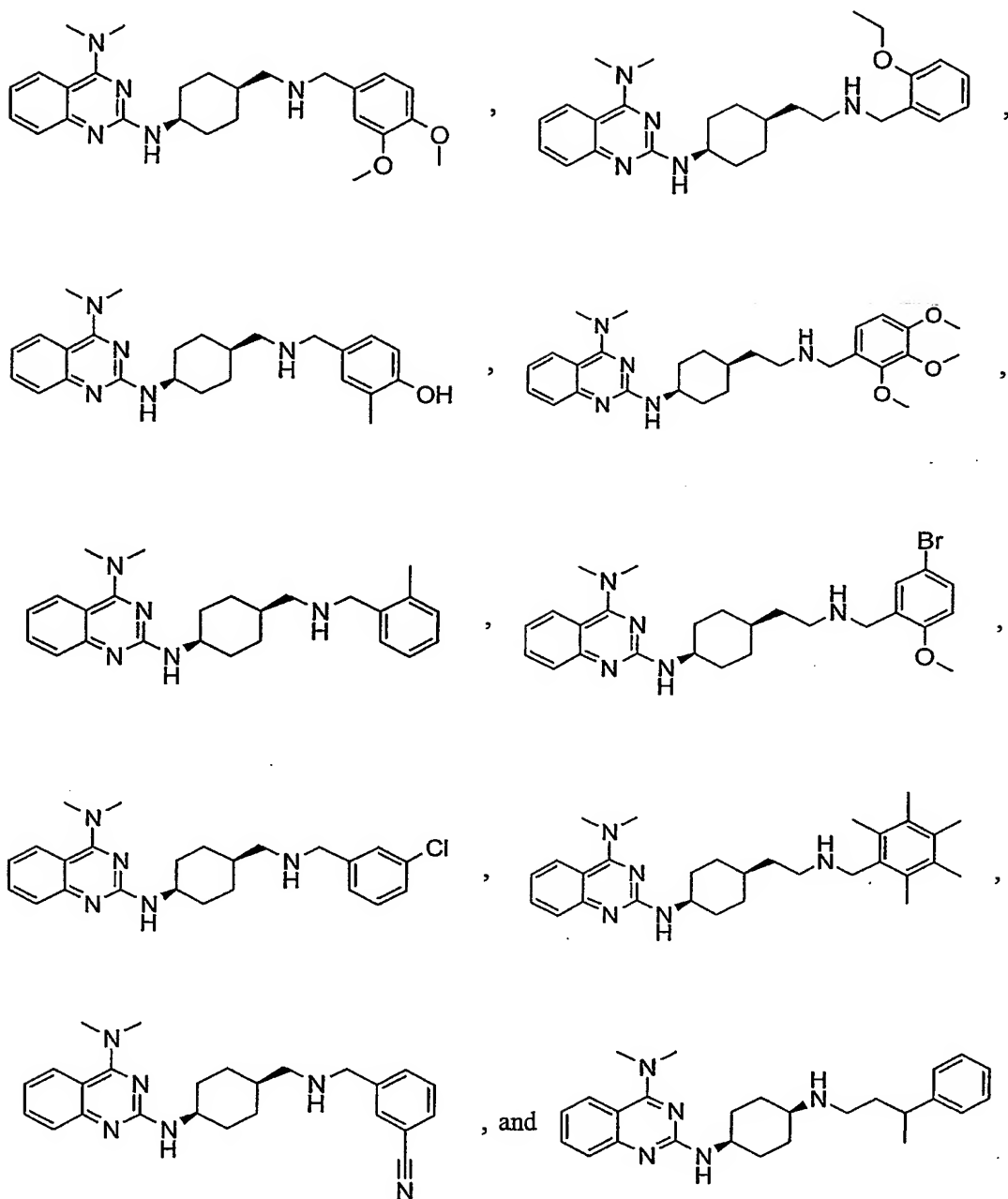












; or, in case of, a salt thereof.

14. A compound according to claim 1, wherein Q is Formula II;

R₁ represents

(i) C₁-C₁₆ alkyl,

C₁-C₁₆ alkyl substituted by substituent(s) independently selected from

•halogen,

•carbocyclyl,

•carbocyclic aryl,

•carbocyclic aryl substituted by substituent(s) independently selected from

••halogen,

••nitro,

••C₁-C₃ alkyl,

••halogenated C₁-C₃ alkyl,

••C₁-C₃ alkoxy,

••halogenated C₁-C₃ alkoxy,

(ii) C₂-C₃ alkenyl,

C₂-C₃ alkenyl substituted by carbocyclic aryl,

(iii) carbocyclic aryl,

carbocyclic aryl substituted by substituent(s) independently selected from

•halogen,

•cyano,

•nitro,

•C₁-C₅ alkyl,

•C₁-C₅ alkyl substituted by substituent(s) independently selected from

••halogen,

••oxo,

•C₂-C₃ alkenyl,

•C₁-C₄ alkoxy,

•C₁-C₄ alkoxy substituted by substituent(s) independently selected from

••halogen,

••heterocyclyl,

••halogenated heterocyclyl,

•carbocyclic aryloxy,

•carbocyclic aryloxy substituted by substituent(s) independently selected from

••halogen,

••nitro,

•heterocyclyloxy,

•heterocyclyloxy substituted by substituent(s) independently selected from

••halogen,

••C₁-C₃ alkyl,

••halogenated C₁-C₃ alkyl,

•C₁-C₃ alkoxy carbonyl,

•mono- or di-C₁-C₄ alkylamino,

•C₁-C₃ alkyl carbonylamino,

•carbocyclic aryl diazo,

•carbocyclic aryl diazo substituted by mono- or di- C₁-C₃ alkylamino,

•C₁-C₃ alkylsulfonyl,

•carbocyclic aryl,

(iv) heterocyclyl,

or heterocyclyl substituted by substituent(s) independently selected from

•halogen,

•C₁-C₃ alkyl,

•C₁-C₃ alkyl substituted by substituent(s) independently selected from

••halogen,

••oxo,

••carbocyclic aryl carbonylamino,

••halogenated carbocyclic aryl carbonylamino,

••heterocyclyl,

••heterocyclyl substituted by substituent(s) independently selected from

•••halogen,

•••C₁-C₃ alkyl,

•••halogenated C₁-C₃ alkyl,

•C₁-C₃ alkoxy,

•C₁-C₃ alkyl carbonylamino,

•carbocyclic arylsulfonyl,

- C₁-C₃ alkoxy carbonyl,
- carbocyclic aryl,
- halogenated carbocyclic aryl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl;

Y is -S(O)₂-;

wherein carbocyclic aryl is phenyl, biphenyl, or naphthyl;

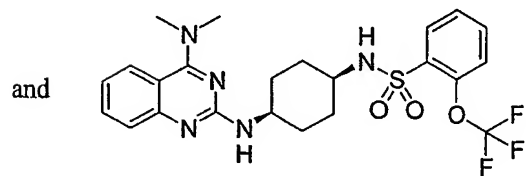
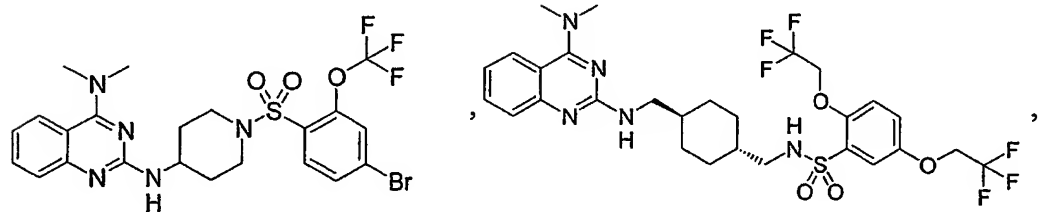
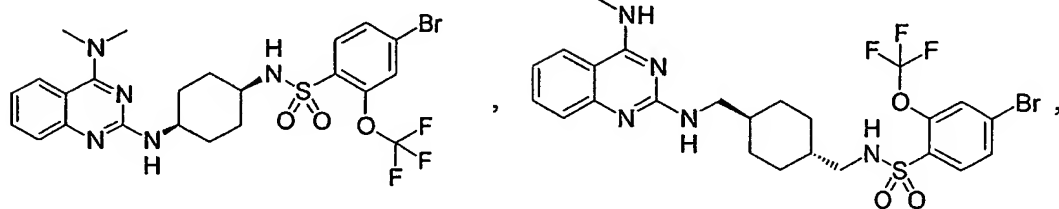
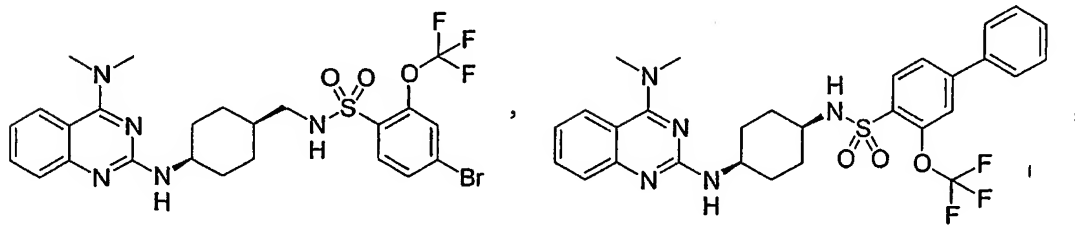
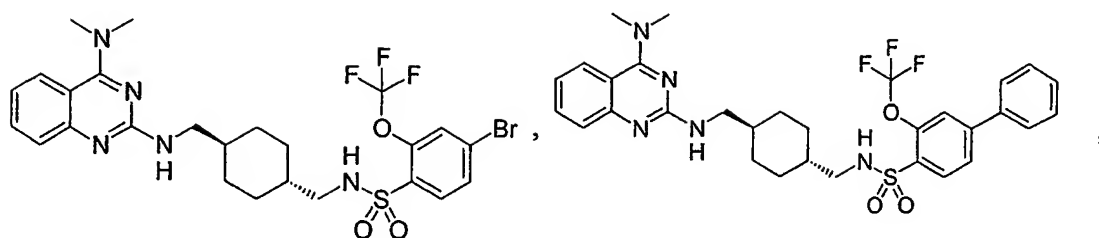
carbocyclyl is 7,7-dimethyl-2-oxo-bicyclo[2.2.1]heptyl;

heterocyclyl is 1,2,3,4-tetrahydro-isoquinolyl, 1,2,3-thiadiazolyl, 1*H*-pyrrolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, furyl, imidazolyl, isoxazolyl, pyrazolyl, pyridyl, quinolyl, thiazolyl, or thienyl;

halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

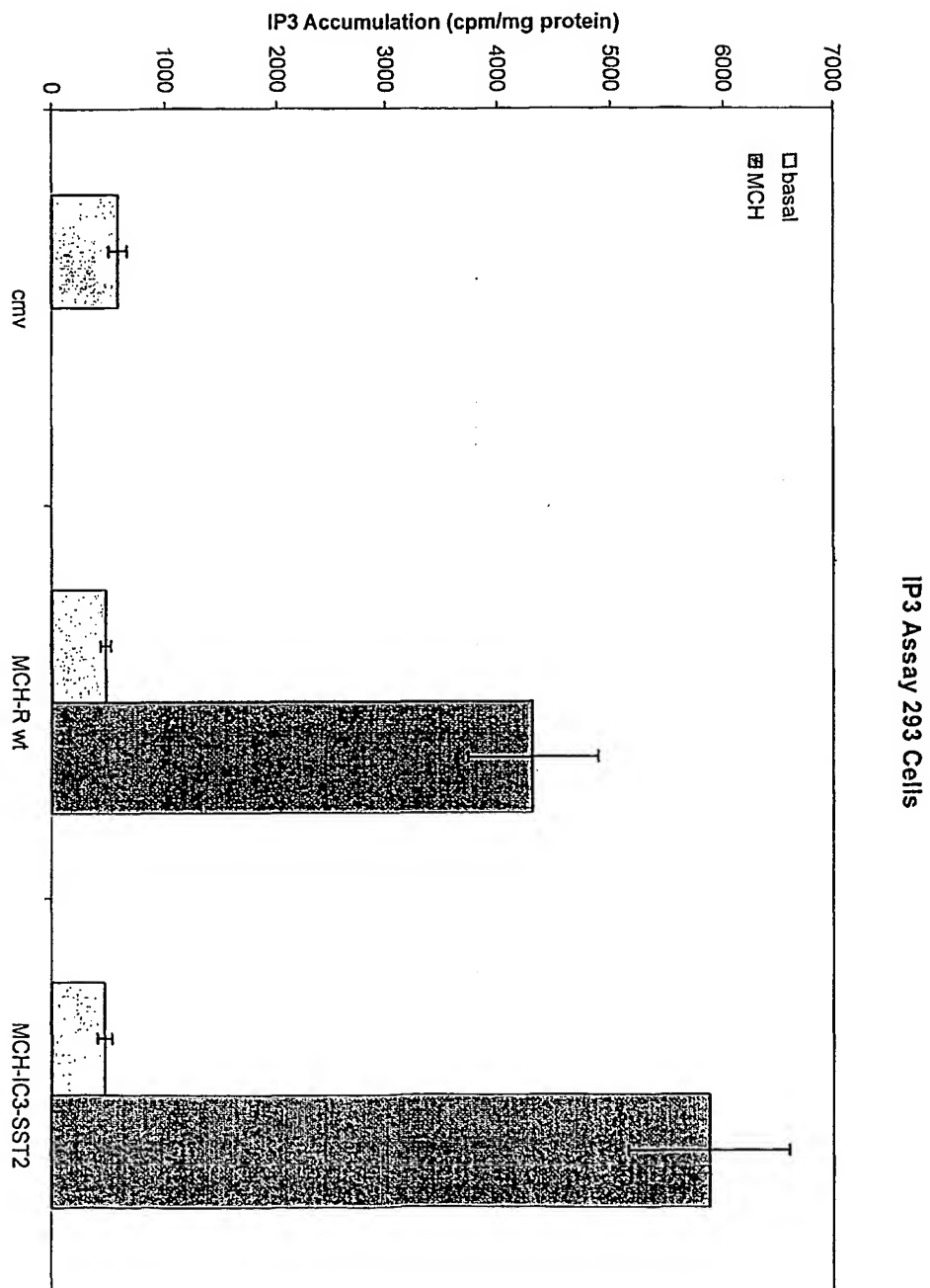
15. A compound according to claim 14 of Formula I selected from the group consisting of



; or, in case of, a salt thereof.

16. A compound according to claim 1, wherein Q is Formula II;
R₁ is selected from H, -CO₂tBu, or -CO₂Bn (Bn is a benzyl group);
R₂ is methylamino or dimethylamino;
L is selected from Formula XX - XXII;
Y is a single bond;
or a salt thereof.
17. A method for modulating the G-protein receptor, SLC-1, comprising the step of contacting said SLC-1 with a MCH receptor antagonist.
18. A method for modulating the G-protein receptor, SLC-1, comprising the step of contacting said SLC-1 with a compound of claims 1-16.
19. The method of prophylaxis or treatment of obesity, obesity related disorders, anxiety, or depression in mammals in need of such treatment comprising administering to the mammal a therapeutically effective amount of a compound having the composition of any of claims 1-16.
20. A pharmaceutical composition comprising a pharmaceutically acceptable carrier and a therapeutically effective amount of a compound having the composition of any of claims 1-16.

Fig. 1



SEQUENCE LISTING

<110> Arena Pharmaceuticals, Inc.

<120> MCH Receptor Antagonists

<130> AREN-0238

<160> 12

<170> PatentIn version 3.0

<210> 1

<211> 30

<212> DNA

<213> Artificial

<220>

<223> Novel Sequence

<400> 1
gtgaagcttg cctctggtgc ctgcaggagg

30

<210> 2

<211> 31

<212> DNA

<213> Artificial

<220>

<223> Novel Sequence

<400> 2

gcagaattcc cggaggcgtg ttgtggtgcc c

31

<210> 3

<211> 24

<212> DNA

<213> Artificial

<220>

<223> Novel Sequence

<400> 3

catgagctgg tggatcatga aggg

24

<210> 4

<211> 24

<212> DNA

<213> Artificial

<220>

<223> Novel Sequence

<400> 4

atgaaggcca tgcccaggag aaag

24

<210> 5

<211> 1349

<212> DNA

<213> Artificial

<220>

<223> Novel Sequence

<400> 5

atggacctgg aagcctcgct gctgccact ggtcccaatg ccagcaacac ctctgatggc

60

cccgataacc tcaacttcggc aggatcacct cctgcacgg ggagcatctc ctacatcaac

120

```

atcatcatgc cttcgggtgtt cggcaccatc tgcctcctgg gcatcatcgg gaactccacg 180
gtcatcttcg cggtcgtgaa gaagtccaag ctgcactggg gcaacaacgt ccccgacatc 240
ttcatcatca acctctcggg agtagatctc ctctttctcc tgggcatgcc cttcatgac 300
caccagctca tgggcaatgg ggtgtggcac tttggggaga ccatgtgcac cctcatcacg 360
gccatggatg ccaatagtca gttcaccagc acctacatcc tgaccgccat ggccattgac 420
cgctacctgg ccaactgtcca ccccatctct tccacgaagt tccggaagcc ctctgtggcc 480
accctgggta tctgcctcct gtgggccctc tccttcatca gcatcacccc tgtgtggctg 540
tatgccagac tcatccctt cccaggagggt gcagtgggct gcggcatacg cctgcccaac 600
ccagacactg acctctactg gttcaccctg taccagtttt tcctggcctt tgccctgcct 660
tttgtggtca tcacagccgc atacgtgagg atcctgcaga aggtgaagtc ctctggaatc 720
cgagtgggct cctctaagag gaagaagtct gagaagaagg tcaccgcac agccatcgcc 780
atctgtctgg tcttctttgt gtgctgggca ccctactatg tgctacagct gacctagt 840
tccatcagcc gcccgacct cacctttgtc tacttataca atgcggccat cagcttgggc 900
tatgccaaca gctgcctcaa cccctttgtg tacatcgtgc tctgtgagac gttccgcaaa 960
cgcttgggtc tgtcggtgaa gcctgcagcc caggggcagc ttgcgcgtgt cagcaacgct 1020
cagacggctg acgaggagag gacagaaagc aaaggcacct gatacttccc ctgccacct 1080
gcacacctcc aagtcagggc accacaacac gccaccggga gagatgctga gaaaaacca 1140
agaccgctcg ggaaatgcag gaaggccggg ttgtgagggg ttgttgcaat gaaataaata 1200
cattccatgg gctcacacgt tgctggggag gcctggagtc aggtttgggg ttttcagata 1260
tcagaaatcc cttgggggag caggatgaga cctttggata gaacagaagc tgagcaagag 1320
aacatgttgg tttggataac cggttgcac 1349

```

<210> 6

<211> 446

<212> PRT

<213> Homo Sapien

<220>

<223> Novel Sequence

<400> 6

Met Asp Leu Glu Ala Ser Leu Leu Pro Thr Gly Pro Asn Ala Ser Asn
 1 5 10 15
 Thr Ser Asp Gly Pro Asp Asn Leu Thr Ser Ala Gly Ser Pro Pro Arg
 20 25 30
 Thr Gly Ser Ile Ser Tyr Ile Asn Ile Ile Met Pro Ser Val Phe Gly
 35 40 45
 Thr Ile Cys Leu Leu Gly Ile Ile Gly Asn Ser Thr Val Ile Phe Ala
 50 55 60
 Val Val Lys Lys Ser Lys Leu His Trp Cys Asn Asn Val Pro Asp Ile
 65 70 75 80
 Phe Ile Ile Asn Leu Ser Val Val Asp Leu Leu Phe Leu Leu Gly Met
 85 90 95
 Pro Phe Met Ile His Gln Leu Met Gly Asn Gly Val Trp His Phe Gly
 100 105 110
 Glu Thr Met Cys Thr Leu Ile Thr Ala Met Asp Ala Asn Ser Gln Phe
 115 120 125
 Thr Ser Thr Tyr Ile Leu Thr Ala Met Ala Ile Asp Arg Tyr Leu Ala
 130 135 140
 Thr Val His Pro Ile Ser Ser Thr Lys Phe Arg Lys Pro Ser Val Ala
 145 150 155 160
 Thr Leu Val Ile Cys Leu Leu Trp Ala Leu Ser Phe Ile Ser Ile Thr
 165 170 175
 Pro Val Trp Leu Tyr Ala Arg Leu Ile Pro Phe Pro Gly Gly Ala Val
 180 185 190
 Gly Cys Gly Ile Arg Leu Pro Asn Pro Asp Thr Asp Leu Tyr Trp Phe
 195 200 205
 Thr Leu Tyr Gln Phe Phe Leu Ala Phe Ala Leu Pro Phe Val Val Ile
 210 215 220
 Thr Ala Ala Tyr Val Arg Ile Leu Gln Lys Val Lys Ser Ser Gly Ile
 225 230 235 240
 Arg Val Gly Ser Ser Lys Arg Lys Lys Ser Glu Lys Lys Val Thr Arg
 245 250 255
 Thr Ala Ile Ala Ile Cys Leu Val Phe Phe Val Cys Trp Ala Pro Tyr
 260 265 270
 Tyr Val Leu Gln Leu Thr Gln Leu Ser Ile Ser Arg Pro Thr Leu Thr
 275 280 285
 Phe Val Tyr Leu Tyr Asn Ala Ala Ile Ser Leu Gly Tyr Ala Asn Ser

290	295	300
Cys Leu Asn Pro Phe Val Tyr Ile Val Leu Cys Glu Thr Phe Arg Lys 305 310 315 320		
Arg Leu Val Leu Ser Val Lys Pro Ala Ala Gln Gly Gln Leu Arg Ala 325 330 335		
Val Ser Asn Ala Gln Thr Ala Asp Glu Glu Arg Thr Glu Ser Lys Gly 340 345 350		
Thr Tyr Phe Pro Cys His Pro Ala His Leu Gln Val Arg Ala Pro Gln 355 360 365		
His Ala Thr Gly Arg Asp Ala Glu Lys Asn Pro Arg Pro Leu Gly Lys 370 375 380		
Cys Arg Lys Ala Gly Leu Gly Val Val Ala Met Lys Ile His Ser Met 385 390 395 400		
Gly Ser His Val Ala Gly Glu Ala Trp Ser Gln Val Trp Gly Phe Gln 405 410 415		
Ile Ser Glu Ile Pro Trp Gly Ser Arg Met Arg Pro Leu Asp Arg Thr 420 425 430		
Glu Ala Glu Gln Glu Asn Met Leu Val Trp Ile Thr Gly Cys 435 440 445		

<210> 7

<211> 70

<212> DNA

<213> Artificial

<220>

<223> Novel Sequence

<400> 7

gatcctgcag aaggtgaagt cctctggaat ccgagtgggc tcctctaaga ggaagaagtc 60

tgagaagaag 70

<210> 8

<211> 71

<212> DNA

<213> Artificial

<220>

<223> Novel Sequence

<400> 8

gtgaccttct tctcagactt cttcctctta gaggagccca ctcggattcc agaggacttc 60

accttctgca g 71

<210> 9

<211> 30

<212> DNA

<213> Artificial

<220>

<223> Novel Sequence

<400> 9

gtgaagcttg cccgggcagg atggacctgg 30

<210> 10

<211> 24

<212> DNA

<213> Artificial

<220>

<223> Novel Sequence

<400> 10

atctagaggt gcctttgctt tctg 24

<210> 11

<211> 2133

<212> DNA

<213> Homo Sapien

<400> 11

atggacctgg aagcctcgct gctgcccact ggtcccaatg ccagcaacac ctctgatggc 60

cccgataacc tcacttcggc aggatcacct cctcgcacgg ggagcatctc ctacatcaac 120

atcatcatgc cttcggtggt cggcaccatc tgcctcctgg gcatcatcgg gaactccacg 180
gtcatcttcg cggtcgtgaa gaagtccaag ctgcaactgg gcaacaacgt ccccgacatc 240
ttcatcatca acctctcggg agtagatctc ctctttctcc tgggcatgcc cttcatgac 300
caccagctca tgggcaatgg ggtgtggcac tttggggaga ccatgtgcac cctcatcacg 360
gccatggatg ccaatagtca gttcaccagc acctacatcc tgaccgcat ggccattgac 420
cgctacctgg ccaactgtcca ccccatctct tccacgaagt tccggaagcc ctctgtggcc 480
acctggtga tctgcctcct gtgggcoctc tccttcatca gcatcacccc tgtgtggctg 540
tatgccagac tcatccctt cccaggagggt gcagtgggct gcggcatacg cctgcccaac 600
ccagacactg acctctactg gttcaccctg taccagtttt tcctggcctt tgccctgcct 660
tttgtggtca tcacagccgc atactgagg atcctgcagc gcatgacgtc ctcagtggcc 720
cccgctccc agcgagcat ccggctgcgg acaaagaggg tgaccgcac agccatcgcc 780
atctgtctgg tcttctitgt gtgctgggca ccctactatg tgctacagct gaccagttg 840
tccatcagcc gcccgacct cacctttgtc tacttataca atgcggccat cagcttgggc 900
tatgccaaca gctgcctcaa cccctttgtg tacatcgtgc tctgtgagac gttccgcaaa 960
cgcttgggtc tgtcgtgaa gcctgcagcc caggggcagc ttcgcgtgt cagcaacgt 1020
cagacggctg acgaggagag gacagaaagc aaaggcacct ctagaatggg ctgcacactg 1080
agcgctgagg acaaggcggc cgtggagcgc agcaagatga tcgaccgcaa cctccgggag 1140
gacggagaga aggcagcggc cgaggtaag ctgctgctgc tgggtgctgg tgaatccggg 1200
aagagcaciaa ttgtgaagca gatgaaaatt atccacgagg ctggctactc agaggaagag 1260
tgtaagcagt acaaagcagt ggtctacagc aacaccatcc agtccatcat tgccatcatt 1320
agagccatgg ggagattgaa aatcgacttt ggagacgctg ctcgtgcgga tgatgctcgc 1380
caactcttcg tgcttgcctg ggctgcagag gaaggcttta tgaccgcgga gctcgccggc 1440
gtcataaaga gactgtggaa ggacagcggg gtgcaagcct gttcaacag atcccgggag 1500
taccagctga acgattcggc ggcgtactac ctgaatgact tggacagaat agcacaacca 1560
aattacatcc caaccagca ggatgttctc agaactagag tgaaaacgac gggaattgtg 1620
gaaaccact ttactttcaa agatcttcat tttaaaatgt ttgacgtggg aggccagaga 1680
tcagagcggg agaagtggat tcaactgctt gaaggcgtga ctgccatcat cttctgtgtg 1740
gccctgagt actatgacct ggttcttgcg gaggatgaag aaatgaaccg gatgcatgaa 1800
agcatgaagc tgttcgatag catatgtaac aacaagtggg ttaaggacac atccatcatc 1860

cttttcctga acaagaagga cctcttcgaa gagaagatca aaaagagtcc cctcacgata 1920
 tgctatccag aatatgcagg ctcaaacaca tatgaagagg cggctgcgta tatccagtgt 1980
 cagtttgaag acctcaataa aaggaaggac acaaaggaaa ttacaccca cttcacttgc 2040
 gccacggata cgaagaatgt gcagtttgtg ttcgatgctg taacggacgt catcataaag 2100
 aataacctaa aagactgtgg tctcttctaa tct 2133

<210> 12
 <211> 709
 <212> PRT
 <213> Homo Sapien

<400> 12
 Met Asp Leu Glu Ala Ser Leu Leu Pro Thr Gly Pro Asn Ala Ser Asn
 1 5 10 15
 Thr Ser Asp Gly Pro Asp Asn Leu Thr Ser Ala Gly Ser Pro Pro Arg
 20 25 30
 Thr Gly Ser Ile Ser Tyr Ile Asn Ile Ile Met Pro Ser Val Phe Gly
 35 40 45
 Thr Ile Cys Leu Leu Gly Ile Ile Gly Asn Ser Thr Val Ile Phe Ala
 50 55 60
 Val Val Lys Lys Ser Lys Leu His Trp Cys Asn Asn Val Pro Asp Ile
 65 70 75 80
 Phe Ile Ile Asn Leu Ser Val Val Asp Leu Leu Phe Leu Leu Gly Met
 85 90 95
 Pro Phe Met Ile His Gln Leu Met Gly Asn Gly Val Trp His Phe Gly
 100 105 110
 Glu Thr Met Cys Thr Leu Ile Thr Ala Met Asp Ala Asn Ser Gln Phe
 115 120 125
 Thr Ser Thr Tyr Ile Leu Thr Ala Met Ala Ile Asp Arg Tyr Leu Ala
 130 135 140
 Thr Val His Pro Ile Ser Ser Thr Lys Phe Arg Lys Pro Ser Val Ala
 145 150 155 160
 Thr Leu Val Ile Cys Leu Leu Trp Ala Leu Ser Phe Ile Ser Ile Thr
 165 170 175
 Pro Val Trp Leu Tyr Ala Arg Leu Ile Pro Phe Pro Gly Gly Ala Val
 180 185 190
 Gly Cys Gly Ile Arg Leu Pro Asn Pro Asp Thr Asp Leu Tyr Trp Phe
 195 200 205

Thr Leu Tyr Gln Phe Phe Leu Ala Phe Ala Leu Pro Phe Val Val Ile
 210 215 220
 Thr Ala Ala Tyr Val Arg Ile Leu Gln Arg Met Thr Ser Ser Val Ala
 225 230 235 240
 Pro Ala Ser Gln Arg Ser Ile Arg Leu Arg Thr Lys Arg Val Thr Arg
 245 250 255
 Thr Ala Ile Ala Ile Cys Leu Val Phe Phe Val Cys Trp Ala Pro Tyr
 260 265 270
 Tyr Val Leu Gln Leu Thr Gln Leu Ser Ile Ser Arg Pro Thr Leu Thr
 275 280 285
 Phe Val Tyr Leu Tyr Asn Ala Ala Ile Ser Leu Gly Tyr Ala Asn Ser
 290 295 300
 Cys Leu Asn Pro Phe Val Tyr Ile Val Leu Cys Glu Thr Phe Arg Lys
 305 310 315 320
 Arg Leu Val Leu Ser Val Lys Pro Ala Ala Gln Gly Gln Leu Arg Ala
 325 330 335
 Val Ser Asn Ala Gln Thr Ala Asp Glu Glu Arg Thr Glu Ser Lys Gly
 340 345 350
 Thr Ser Arg Met Gly Cys Thr Leu Ser Ala Glu Asp Lys Ala Ala Val
 355 360 365
 Glu Arg Ser Lys Met Ile Asp Arg Asn Leu Arg Glu Asp Gly Glu Lys
 370 375 380
 Ala Ala Arg Glu Val Lys Leu Leu Leu Leu Gly Ala Gly Glu Ser Gly
 385 390 395 400
 Lys Ser Thr Ile Val Lys Gln Met Lys Ile Ile His Glu Ala Gly Tyr
 405 410 415
 Ser Glu Glu Glu Cys Lys Gln Tyr Lys Ala Val Val Tyr Ser Asn Thr
 420 425 430
 Ile Gln Ser Ile Ile Ala Ile Ile Arg Ala Met Gly Arg Leu Lys Ile
 435 440 445
 Asp Phe Gly Asp Ala Ala Arg Ala Asp Asp Ala Arg Gln Leu Phe Val
 450 455 460
 Leu Ala Gly Ala Ala Glu Glu Gly Phe Met Thr Ala Glu Leu Ala Gly
 465 470 475 480
 Val Ile Lys Arg Leu Trp Lys Asp Ser Gly Val Gln Ala Cys Phe Asn
 485 490 495
 Arg Ser Arg Glu Tyr Gln Leu Asn Asp Ser Ala Ala Tyr Tyr Leu Asn
 500 505 510

Asp Leu Asp Arg Ile Ala Gln Pro Asn Tyr Ile Pro Thr Gln Gln Asp
 515 520 525
 Val Leu Arg Thr Arg Val Lys Thr Thr Gly Ile Val Glu Thr His Phe
 530 535 540
 Thr Phe Lys Asp Leu His Phe Lys Met Phe Asp Val Gly Gly Gln Arg
 545 550 555 560
 Ser Glu Arg Lys Lys Trp Ile His Cys Phe Glu Gly Val Thr Ala Ile
 565 570 575
 Ile Phe Cys Val Ala Leu Ser Asp Tyr Asp Leu Val Leu Ala Glu Asp
 580 585 590
 Glu Glu Met Asn Arg Met His Glu Ser Met Lys Leu Phe Asp Ser Ile
 595 600 605
 Cys Asn Asn Lys Trp Phe Thr Asp Thr Ser Ile Ile Leu Phe Leu Asn
 610 615 620
 Lys Lys Asp Leu Phe Glu Glu Lys Ile Lys Lys Ser Pro Leu Thr Ile
 625 630 635 640
 Cys Tyr Pro Glu Tyr Ala Gly Ser Asn Thr Tyr Glu Glu Ala Ala Ala
 645 650 655
 Tyr Ile Gln Cys Gln Phe Glu Asp Leu Asn Lys Arg Lys Asp Thr Lys
 660 665 670
 Glu Ile Tyr Thr His Phe Thr Cys Ala Thr Asp Thr Lys Asn Val Gln
 675 680 685
 Phe Val Phe Asp Ala Val Thr Asp Val Ile Ile Lys Asn Asn Leu Lys
 690 695 700
 Asp Cys Gly Leu Phe
 705